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Bis(propane-1,3-diaminium) benzene-1,2,4,5-tetracarboxylate dihydrate

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The title salt, $(PnH_2)_2(Btc)\cdot 2H_2O$ or $2C_3H_{12}N_2^{2+}\cdot C_{10}H_2O_8^{4-}\cdot$-$2H_2O$, has been prepared from propane-1,3-diamine (Pn) and benzene-1,2,4,5-tetracarboxylic acid ($BtcH_4$). A wide range of noncovalent interactions, consisting of ion pairing and hydrogen bonding with $D\cdots A$ distances ranging from 2.7075 (15) to 2.9726 (15) Å, connect the various components into a supramolecular structure.

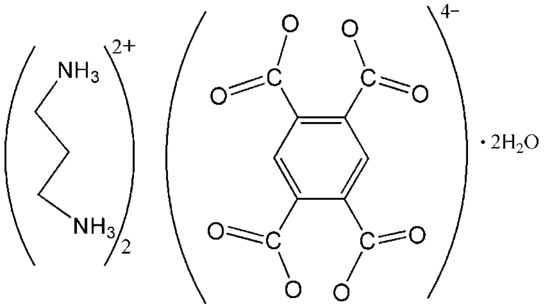
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.068
Data-to-parameter ratio = 10.7

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

Comment

The preparation and characterization of proton-transfer compounds have been considered by chemists in recent years. Our research group has recently focused on the synthesis of new systems that can act as suitable ligands in the synthesis of organometal complexes (Aghabozorg, Ghasemikhah *et al.*, 2006; Aghabozorg, Aghajani & Sharif, 2006). In our previous work, 1,10-phenanthroline (Phen) and its derivatives act as chelating ligands to a central atom (Aghabozorg *et al.*, 2005; Sheshmani *et al.*, 2006) or participate in proton-transfer systems such as $(PhenH)_2(BtcH_3)(BtcH_2)_{0.5}$ ($BtcH_4$ is benzene-1,2,4,5-tetracarboxylic acid; Aghabozorg, Ghadermazi, Attar Gharamaleki 2006), $(PhenH)_2(Pydc)$ ($PydcH_2$ is pyridine-2,6-dicarboxylic acid; Moghimi *et al.*, 2005) and $(CreatH)(Phendc)\cdot H_2O$ (Creat is creatinine and $PhendcH_2$ is 1,10-phenanthroline-2,9-dicarboxylic acid; Soleimannejad *et al.*, 2005). We report here a proton-transfer system containing benzene-1,2,4,5-tetracarboxylic acid and propane-1,3-diamine.



(I)

The asymmetric unit of the title compound, (I), consists of a stoichiometric 1:2 salt triad plus two water molecules, as shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

The crystal structure of (I) shows that all H atoms are transferred from the carboxyl groups to the N atoms of the propane-1,3-diamine molecules.

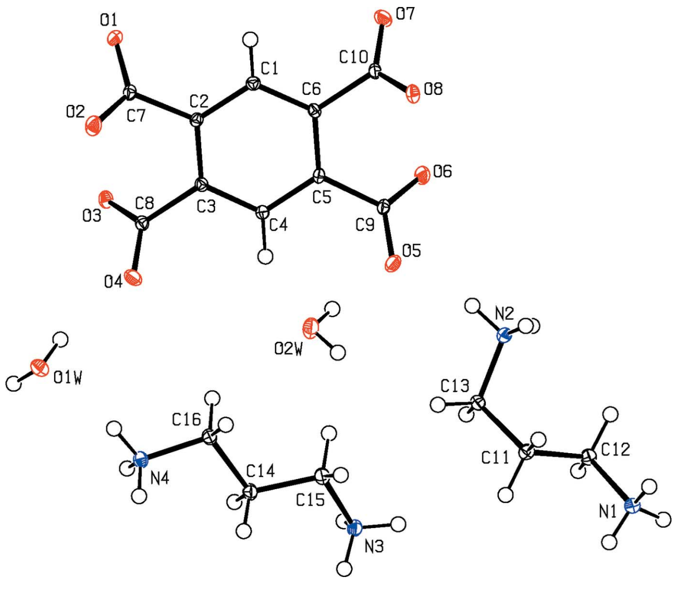


Figure 1
The asymmetric unit of $(PnH_2)_2(Btc)\cdot 2H_2O$, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

A number of O—H···O, N—H···O and C—H···O hydrogen bonds, with *D*···*A* distances ranging from 2.7075 (15) to 2.9726 (15) Å, are observed in the crystal structure of (I) (Table 1), producing a three-dimensional network which results in the formation of a supramolecular structure. Ion pairing and van der Waals interactions are also effective in the packing of the crystal structure.

Experimental

The reaction of benzene-1,2,4,5-tetracarboxylic acid (10 mmol, 2.54 g) in tetrahydrofuran (THF; 20 ml) with propane-1,3-diamine (20 mmol, 1.48 g) in THF (20 ml) led to the formation of a colourless precipitate, which was filtered off and dried. The resulting powder was dissolved in water to give colourless crystals of compound (I) after four weeks at room temperature.

Crystal data

$2C_3H_{12}N_2^{2+}\cdot C_{10}H_2O_8^{4-}\cdot 2H_2O$
$M_r = 438.44$
Monoclinic, $P2_1$
$a = 6.9869\ (3)$ Å
$b = 18.3967\ (8)$ Å
$c = 8.2995\ (4)$ Å
$\beta = 113.617\ (1)^\circ$
$V = 977.43\ (8)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 100\ (2)$ K
0.5 × 0.4 × 0.3 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: none
10346 measured reflections
2912 independent reflections
2855 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.068$
$S = 1.03$
2912 reflections
271 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.39$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.22$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*NA*···O3$^{\rm i}$	0.90	1.96	2.8512 (16)	173
N1—H1*NB*···O1$^{\rm ii}$	0.90	1.94	2.8409 (16)	174
N1—H1*NC*···O7$^{\rm iii}$	0.90	2.15	2.9145 (15)	142
N1—H1*NC*···O1*W*$^{\rm iv}$	0.90	2.46	2.9726 (15)	117
N2—H2*NA*···O3$^{\rm ii}$	0.90	1.96	2.8379 (15)	166
N2—H2*NB*···O5	0.90	1.86	2.7257 (16)	161
N2—H2*NC*···O8$^{\rm v}$	0.90	1.93	2.8154 (15)	167
N3—H3*NA*···O2*W*$^{\rm v}$	0.90	1.98	2.7618 (17)	145
N3—H3*NB*···O4$^{\rm v}$	0.90	1.88	2.7664 (15)	167
N3—H3*NC*···O1$^{\rm iii}$	0.90	1.86	2.7455 (15)	165
N4—H4*NA*···O1*W*	0.90	1.98	2.8418 (17)	161
N4—H4*NB*···O8$^{\rm vi}$	0.90	1.85	2.7481 (15)	174
N4—H4*NC*···O3$^{\rm vii}$	0.90	2.02	2.9200 (14)	173
O1*W*—H1*WA*···O6$^{\rm vi}$	0.85	1.87	2.7075 (15)	170
O1*W*—H1*WB*···O4	0.85	1.97	2.7454 (14)	151
O2*W*—H2*WA*···O7$^{\rm vii}$	0.85	1.89	2.7299 (15)	173
O2*W*—H2*WB*···O5	0.85	1.94	2.7800 (15)	170

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

All H atoms were found in a difference Fourier synthesis and were treated using an isotropic riding-model approximation, with C—H = 0.95–0.99 Å, N—H = 0.90 Å and O—H = 0.85 Å, and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C,N,O). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; 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*.

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