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## Key indicators

Single-crystal X-ray study  
 $T = 291$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.099  
Data-to-parameter ratio = 14.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2,2'-Dihydroxy-3,3'-(piperazinedium-  
1,4-diyl)bis(propanesulfonate) dihydrateThe buffer reagent piperazine-1,4-diylbis(2-hydroxypropane-  
sulfonic acid) (PBHPS), when crystallized from an aqueous  
solution, exists as the title centrosymmetric hydrated zwitter-  
tion,  $\text{C}_{10}\text{H}_{22}\text{N}_2\text{O}_8\text{S}_2 \cdot 2\text{H}_2\text{O}$ . The zwitterion and solvent water  
molecules are linked by hydrogen bonds into a three-  
dimensional network.Received 13 July 2006  
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## Comment

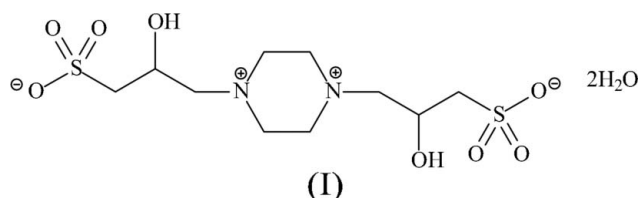
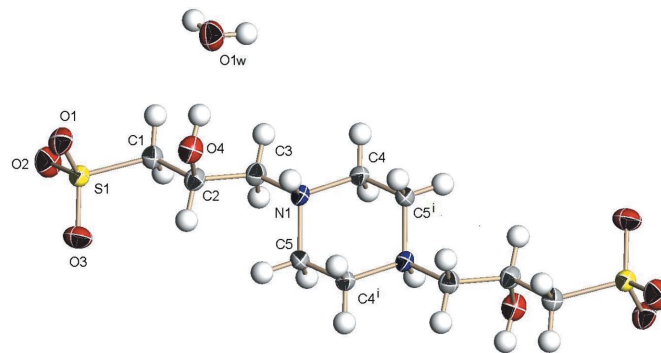
Piperazine-1,4-diylbis(2-hydroxypropanesulfonic acid),  
abbreviated PBHPS, is used as a buffer (Mash *et al.*, 2003;  
Wiedmer *et al.*, 2005), the crystal structure of which has not  
been reported to date. The compound exists as a centrosym-  
metric dihydrated piperazinium-1,4-bis(2-hydroxypropyl-  
sulfonate) zwitterion, (I) (Fig. 1). The six-membered  
piperazinium ring adopts the common chair conformation and  
the two 2-hydroxypropylsulfonate substituents occupy equa-  
torial positions. The structure is stabilized by extensive  
hydrogen-bonding interactions which give rise to a three-  
dimensional network (Table 1).Another piperazine-sulfonate type of buffer, 4-(2-  
hydroxyethyl)-1-piperazineethylsulfonic acid (HEPES), also  
exists as a zwitterionic molecule that interacts with adjacent  
zwitterions, but the hydrogen bonds lead to a sheet structure

Figure 1

The structure of (I). Displacement ellipsoids are drawn at the 50%  
probability level, and H atoms are shown as spheres of arbitrary radii.  
The di-zwitterion lies on a centre of inversion [symmetry code: (i)  $1 - x,$   
 $1 - y, 1 - z$ .]

(Wouters *et al.*, 1996). A second orthorhombic HEPES polymorph is also known, in which the H atom was found to be bonded to the sulfonate group (Gao *et al.*, 2004).

## Experimental

Commercially available piperazine-1,4-diylbis(2-hydroxypropane-sulfonic acid) (0.38 g, 1.0 mmol) was dissolved in methanol (15 ml). The pH of the solution was adjusted to about 7.5 by the addition of drops of hydrochloric acid. The clear solution was set aside for a week for crystals of (I) to form.

### Crystal data

$C_{10}H_{22}N_2O_8S_2 \cdot 2H_2O$   
 $M_r = 398.45$   
 Monoclinic,  $P2_1/n$   
 $a = 8.6675$  (8) Å  
 $b = 7.2050$  (6) Å  
 $c = 13.198$  (1) Å  
 $\beta = 96.859$  (1)°  
 $V = 818.31$  (12) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.617$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.38$  mm<sup>-1</sup>  
 $T = 291$  (2) K  
 Block, colourless  
 $0.21 \times 0.14 \times 0.05$  mm

### Data collection

Bruker APEXII area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 4919 measured reflections

1865 independent reflections  
 1551 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.021$   
 $\theta_{max} = 27.5^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.099$   
 $S = 1.03$   
 1865 reflections  
 125 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.5041P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.24$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O4—H4O <sup>i</sup> ···O1W	0.85 (1)	1.89 (1)	2.732 (3)	174 (2)
O1W—H1W2···O2 <sup>i</sup>	0.84 (1)	1.90 (2)	2.698 (2)	157 (3)
O1W—H1W1···O4 <sup>ii</sup>	0.84 (1)	2.28 (3)	2.824 (2)	123 (3)
N1—H1N···O1 <sup>ii</sup>	0.85 (1)	2.09 (2)	2.834 (2)	147 (2)

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

Carbon-bound H atoms were positioned geometrically ( $C-H = 0.97$  and  $0.98$  Å) and were included in the refinement in the riding-model approximation, with  $U_{iso}(H) = 1.2U_{eq}(C)$ . The ammonium and water H atoms were located in a difference Fourier map and were refined with a distance restraint of  $N-H = O-H = 0.85$  (1) Å.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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## References

- Bruker (2004). *SAINT* (Version 7.12A), *SHELXTL* (Version 5) and *SMART* (Version 7.12A). Bruker AXS Inc., Madison, Wisconsin, USA.
- Gao, F., Yin, C.-X., Yang, P. & Xue, G. (2004). *Acta Cryst.* **E60**, o1328–o1329.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Mash, H. E., Chin, Y.-P., Sigg, L., Hari, R. & Xue, H.-B. (2003). *Anal. Sci.* **75**, 671–677.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wiedmer, S. K., Jussila, M., Hakala, R. M. S., Pystynen, K.-H. & Riekkola, M.-L. (2005). *Electrophoresis*, **26**, 1920–1927.
- Wouters, J., Häming, L. & Sheldrick, G. (1996). *Acta Cryst.* **C52**, 1687–1688.