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## Key indicators

Single-crystal X-ray study  
 $T = 103\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.033  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 18.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

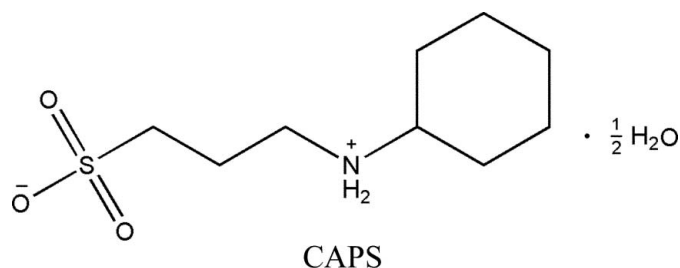
## 3-Cyclohexylaminopropane-1-sulfonic acid hemihydrate

The biological buffer 3-cyclohexylaminopropane-1-sulfonic acid (CAPS,  $\text{C}_9\text{H}_{19}\text{NO}_3\text{S}$ ) crystallizes in the space group  $C2/c$  with two CAPS molecules and one water molecule in the asymmetric unit. As is the case for other aminosulfonic acids, CAPS is a zwitterion. Molecules are linked into hydrogen-bonded dimers by interactions involving one of the amine protons and sulfonic acid O atoms, and these dimers are further linked through hydrogen bonding *via* the water molecule to form layers. These layers are linked by out-of-plane hydrogen bonds involving the other amine proton.

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## Comment

CAPS (3-cyclohexylaminopropane-1-sulfonic acid) is a widely used (Zaitseva *et al.*, 2004) biological buffer ( $\text{p}K_a = 10.4$ ; Roy *et al.*, 1997) presenting a useful pH range between 9.8 and 11.0. As is commonly found for aminosulfonic acids (Wouters & Stalke, 1996; Kim *et al.*, 1979, 1973*a,b*; Doi *et al.*, 1983; Yokoyama *et al.*, 2003; Clarke & Steward, 1977; Ueoka *et al.*, 1972), CAPS crystallizes as a zwitterion with the acid proton transferred to the N atom.



There are two CAPS molecules and a water molecule in the asymmetric unit (Fig. 1) in space group  $C2/c$ . Each CAPS molecule adopts an extended conformation and exhibits S—O bond lengths that are inequivalent (Table 1). In each molecule there is one long (S1A—O3A, S1B—O3B) and two short (S1A—O1A, S1A—O2A; S1B—O1B, S1B—O2B) S—O bond lengths. Both O3A and O3B, which form longer S—O bonds, participate in two intermolecular hydrogen bonds with amine protons (Table 2), while the remaining O atoms either participate in one hydrogen bond with the water molecule (O2A and O1B) or one hydrogen bond with the remaining amine H (O1A and O2B). Through these interactions, CAPS molecules form dimers *via* N—H $\cdots$ O hydrogen bonds and these dimers are further linked in the  $ac$  plane through hydrogen bonds to the water molecule (Fig. 2). Layers in the  $ac$  plane are linked into a three-dimensional network by out-of-plane N—H $\cdots$ O hydrogen bonds (Fig. 3).

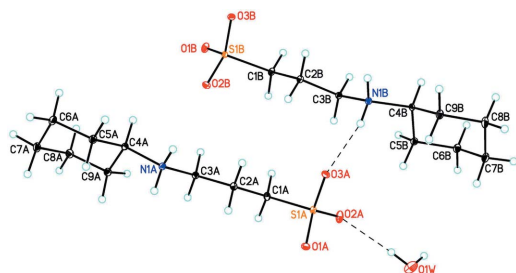


Figure 1

The asymmetric unit of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms. Dashed lines denote hydrogen bonds.

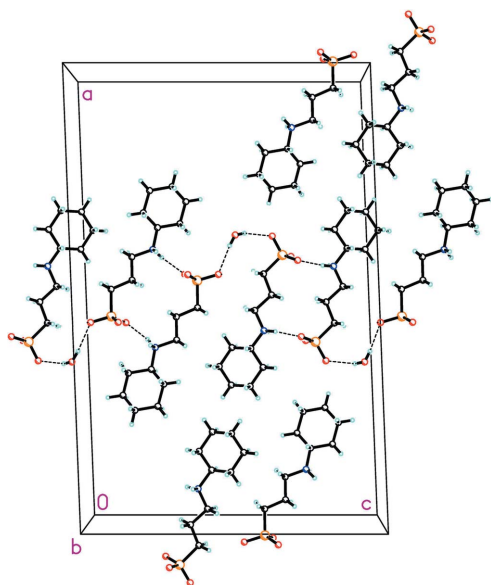


Figure 2

View of part of an extended layer in the *ac* plane, showing dimers formed by N—H...O hydrogen bonds, linked by O—H...O hydrogen bonds through the water molecules (hydrogen bonds are shown as dashed lines).

## Experimental

A buffer solution was prepared by dissolving 11.02 g of CAPS in 50 ml of water and sufficient 3 M NaOH solution to reach a final pH of 10.00. On storage overnight, colorless crystals formed.

### Crystal data

$C_9H_{19}NO_3S \cdot 0.5H_2O$   
 $M_r = 230.32$   
 Monoclinic,  $C2/c$   
 $a = 29.2675$  (17) Å  
 $b = 8.1613$  (4) Å  
 $c = 19.0984$  (11) Å  
 $\beta = 92.206$  (2)°  
 $V = 4558.5$  (4) Å<sup>3</sup>

$Z = 16$   
 $D_x = 1.342$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.27$  mm<sup>-1</sup>  
 $T = 103$  (2) K  
 Block, colorless  
 $0.59 \times 0.25 \times 0.20$  mm

### Data collection

Bruker APEX-II CCD diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.855$ ,  $T_{max} = 0.947$

20375 measured reflections  
 4813 independent reflections  
 4297 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.028$   
 $\theta_{max} = 26.7^\circ$

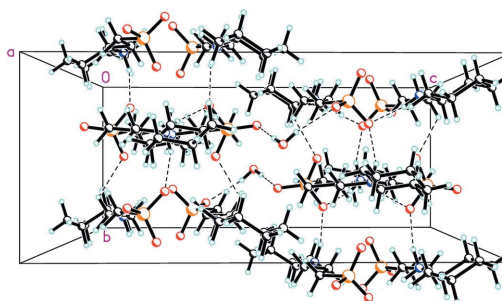


Figure 3

View down the *a* axis, showing out-of-plane N—H...O hydrogen bonds (dashed lines).

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.085$   
 $S = 1.04$   
 4813 reflections  
 268 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 4.8323P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.39$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

S1A—O1A	1.4515 (11)	S1B—O1B	1.4514 (10)
S1A—O2A	1.4528 (10)	S1B—O2B	1.4527 (11)
S1A—O3A	1.4745 (10)	S1B—O3B	1.4769 (10)
S1A—C1A	1.7842 (13)	S1B—C1B	1.7785 (13)
N1A—C3A	1.4894 (17)	N1B—C3B	1.4944 (16)
N1A—C4A	1.5093 (16)	N1B—C4B	1.5066 (16)
O1A—S1A—O2A	114.26 (7)	O1B—S1B—O2B	114.69 (7)
O1A—S1A—O3A	111.13 (6)	O1B—S1B—O3B	112.36 (6)
O2A—S1A—O3A	112.56 (6)	O2B—S1B—O3B	110.84 (6)
O1A—S1A—C1A	107.10 (6)	O1B—S1B—C1B	105.43 (6)
O2A—S1A—C1A	105.38 (6)	O2B—S1B—C1B	107.23 (6)
O3A—S1A—C1A	105.70 (6)	O3B—S1B—C1B	105.59 (6)
C3A—N1A—C4A	117.44 (10)	C3B—N1B—C4B	116.89 (10)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1W1...O2A	0.832 (16)	2.108 (16)	2.9354 (17)	173 (3)
O1W—H1W2...O1B <sup>i</sup>	0.829 (16)	2.181 (17)	2.9821 (18)	162 (2)
N1A—H1AC...O3A <sup>ii</sup>	0.92	1.99	2.8924 (15)	165
N1A—H1AD...O3B <sup>iii</sup>	0.92	1.96	2.8243 (16)	155
N1A—H1AD...O1A <sup>ii</sup>	0.92	2.58	3.0721 (15)	114
N1B—H1BC...O3A	0.92	2.00	2.8453 (16)	152
N1B—H1BC...O2B <sup>ii</sup>	0.92	2.60	3.0747 (15)	113
N1B—H1BD...O3B <sup>ii</sup>	0.92	1.92	2.8253 (15)	167

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

All H atoms were visible in a difference Fourier map. The C—H distances were constrained to an ideal geometry (0.99 Å for CH<sub>2</sub>, and 1.00 Å for CH), and allowed to ride during subsequent refinement, with  $U_{iso}(H) = 1.2U_{eq}(C)$ . The N—H distances were normalized to

0.92 Å, and then the H atoms were allowed to ride with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ . The positions of the H atoms of the water molecule were refined, with O–H restrained to be 0.82 (2) Å, H··H restrained to be 1.30 (2) Å, and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Bruker 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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