SUPPORTING INFORMATION

Sulfamethoxazoles salts: crystal structures, conformations and solubility

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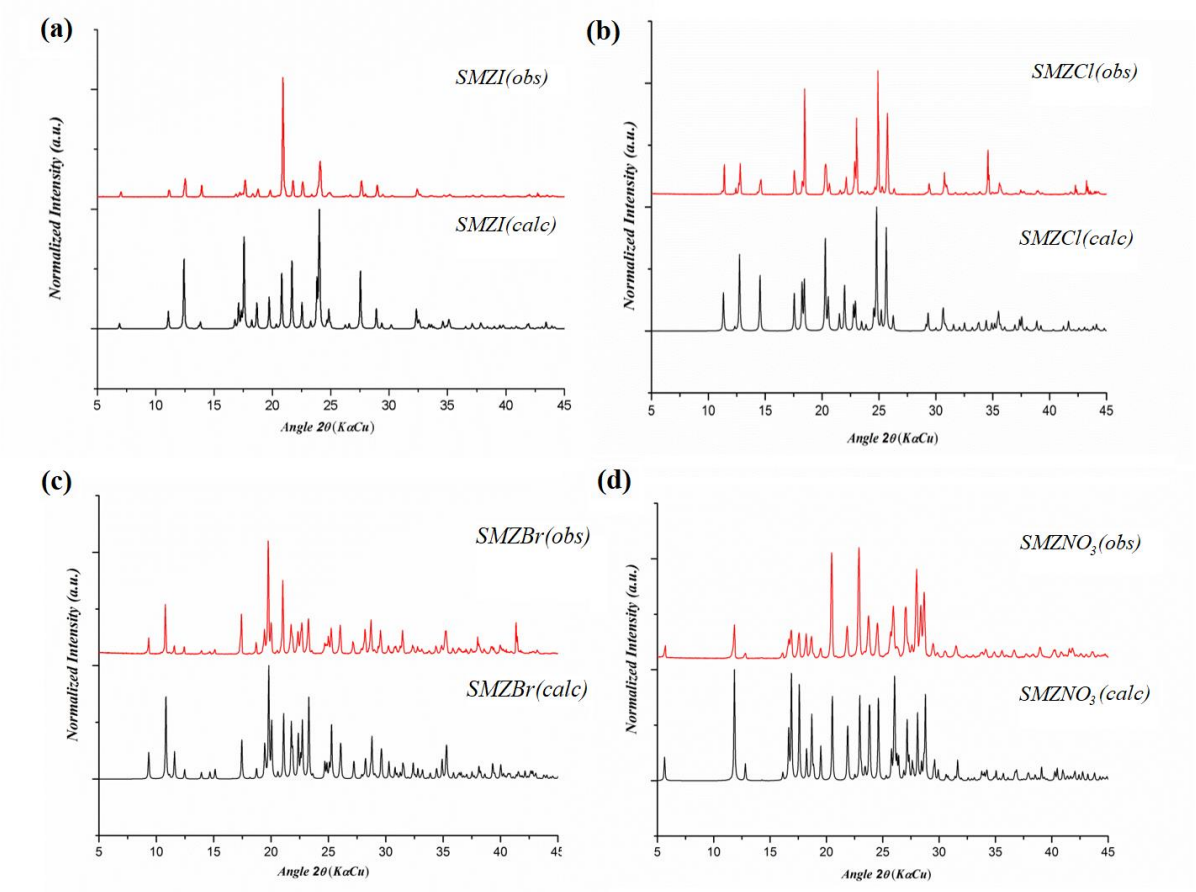

Figure S1: PXRD data for polymorph I of sulfamethoxazole (a), sulfamethoxazole chloride (b), sulfamethoxazole bromide (c) and sulfamethoxazole nitrate (d). For all samples, the experimental and calculated PXRD patterns show a good agreement, thus proving the purity of the samples.

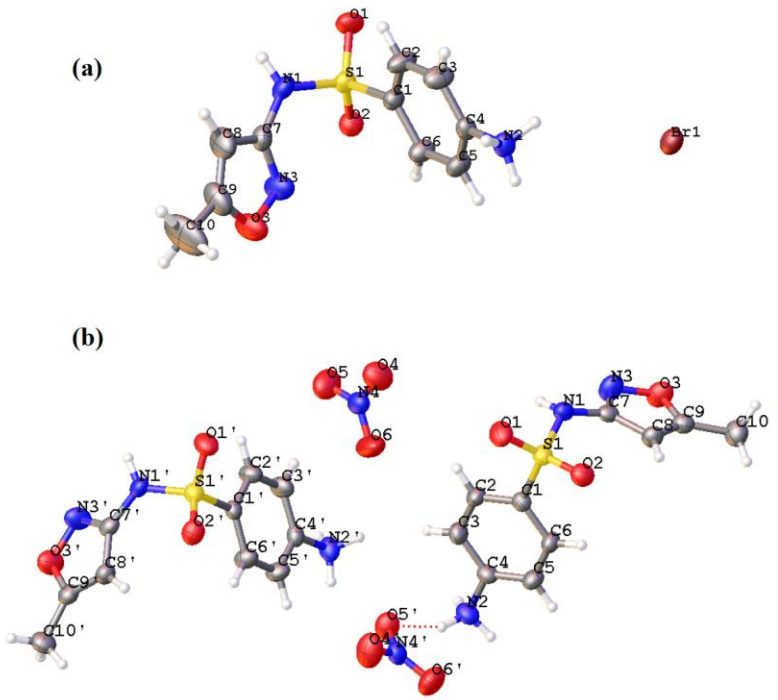

Figure S2: ORTEP view of the asymmetric unit in the sulfamethoxazole salts: bromide (a) and nitrate (b). Thermal ellipsoids for non-hydrogen atoms are drawn at 50% probability level.

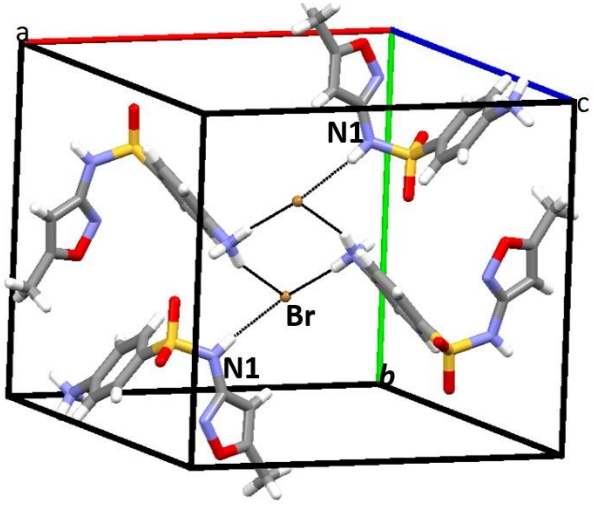

Figure S3: View of the 3D packing of sulfamethoxazole bromide.

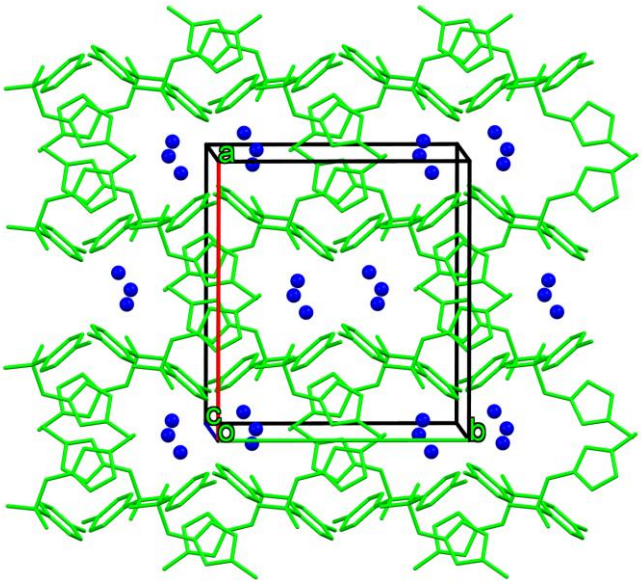

Figure S4: View of the overall assembly characterized by formation of channels along the c-axis that are occupied by the bromide anions. SMX+ cations and bromide anions in green capped sticks and blue ball, respectively. H atoms were omitted for clarity.

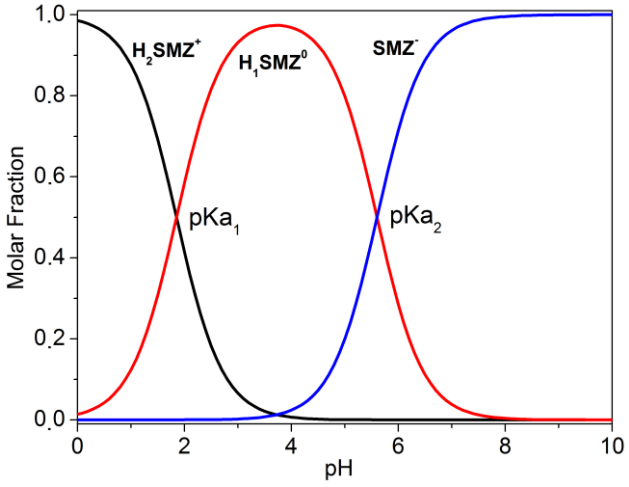

Figure S5: The calculated pH-dependent acid–base SMZ species distribution. $\alpha_2 = [H_2SMZ^+]/C = (1 + (Ka_1/[H^+]) + (Ka_1 \times Ka_2/[H^+]^2))^{-1}$; $\alpha_1 = [H_1BMZ^0]/C = \alpha_2(Ka_1/[H^+])$; $\alpha_0 = [BMZ^-]/C = \alpha_2(Ka_1 \times Ka_1/[H^+]^2)$; where $\alpha_0 + \alpha_1 + \alpha_2 = 1$ and $C = [H_2SMZ^+] + [H_1BMZ^0] + [BMZ^-]$. Curves show pH in steps of 0.1.

Table S1. Geometric parameters of the hydrogen bonds in the SMZ salts

Interaction	D···H(Å)	D···A(Å)	H···A(Å)	D-H···A(º)	Symmetry code
SMZBr					
N1–H1•••Br^-	0.86	3.3438(2)	2.49	173	-x,y,1/2-z
$N2^+$–H2A•••Br^-	0.89	3.4334(2)	2.59	158	1/2+x,1/2+y,z
$N2^+$–H2B•••O2	0.89	2.9172(2)	2.46	112	x,1-y,-1/2+z
$N2^+$–H2B•••N3	0.89	2.9062(2)	2.05	160	x,1-y,-1/2+z
$N2^+$–H2C•••Br^-	0.89	3.2570(2)	2.37	173	1/2-x,1/2-y,-z
$SMZNO_3$					
$N2^+$–H2B•••$O5^-$	0.89	2.9151(2)	2.33	123	1+x,y,-1+z
$N2^+$–H2B•••$O4^-$	0.89	2.9860(2)	2.19	149	1+x,y,-1+z
$N2^+$–H2A•••$O4^-$	0.89	2.8844(2)	2.00	170	x,y,-1+z
$N2^+$–H2B•••$O1^-$	0.89	2.9749(2)	2.42	121	x,y,-1+z
N1-H1•••O2	0.86	3.0931(2)	2.35	144	-1+x,y,z
C8-H8•••N3	0.93	3.2045(2)	2.39	146	1+x,y,z
$N2'^+$–H2B•••$O4'^-$	0.89	3.0401(2)	2.27	145	x,y,z
$N2'^+$–H2B•••$O5'^-$	0.89	2.9092(2)	2.29	126	x,y,z
$N2'^+$–H2A•••$O4'^-$	0.89	2.8098(2)	1.93	168	-1+x,y,z
$N2'^+$–H2B•••$O1'^-$	0.89	2.9413(2)	2.35	124	x,y,z-1
N1'-H1•••O2'	0.86	3.1028(2)	2.30	155	-1+x,y,z
C8'-H8•••N3'	0.93	3.1962(2)	2.39	145	1+x,y,z
$N2^+$–H2C•••$O5'^-$	0.89	2.8028(2)	1.98	152	x,y,z