Electronic Supplementary Material (ESI) for CrystEngComm.

Table S1. Crystal data, data collection and structure refinement parameters for crystal structures of **I**, **II** and **III**.

Crystal structure	**I**	**II**	**III**
Chemical formula	$C_4H_{11}NO_4$	$C_4H_{11}NO_5$	$C_4H_9NO_3$
M_r	137.14	153.14	119.12
Crystal system	orthorhombic	orthorhombic	monoclinic
Space group	$Pca2_1$	$P2_12_12$	$P2_1/n$
Crystal size / mm	0.35x0.3x0.1	0.3 x 0.1 x 0.1	0.3x0.25x0.09
a/Å	10.3838(5)	12.3320(4)	5.5044(7)
b/Å	5.7184(3)	9.9903(3)	10.0817(8)
c/Å	11.4118(7)	5.80218(16)	10.2203(13)
β (°)	90	90	93.142(10)
V/Å^3	677.62(6)	714.83(3)	566.31(11)
Z, Z'	4, 1	4, 1	4, 1
D_{calc}/g cm^{-3}	1.344	1.423	1.397
μ/mm^{-1}	0.120	0.131	0.119
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7718 1383 997	11656 1782 1650	5300 1406 1061
θ_{min} (°)	3.56	2.62	2.84
θ_{max} (°)	26.37	28.28	28.28
Range of			
h	-12 → 12	-16 → 16	-7 → 7
k	-7 → 7	-13 → 13	-13 → 13
l	-14 → 14	-7 → 7	-13 → 13
R_{int}	0.0566	0.0247	0.0273
$R[F^2 > 2\sigma(F^2)]$	0.0415	0.0308	0.0376
$wR(F^2)$	0.0806	0.0777	0.0971
S	1.058	1.043	1.032
No of parameters	93	102	77
Restraints	1	0	0
$\Delta\rho_{max}$/eÅ^{-3}	0.103	0.199	0.202
$\Delta\rho_{min}$/eÅ^{-3}	-0.118	-0.118	-0.187

Figure S1. The main structural motif ("hollow tube") in N-hydroxy-N,N-dimethylglycine perhydrate (**II**). Zigzgag chains are highlighted by red and blue, O3-H3O...O4 hydrogen bond is highlighted by green. Intramolecular O3-H3O...O1 hydrogen bond is omitted for clarity.