Electronic supplementary information

Effect of pressure on slit channels in guaninine sodium salt hydrate: a link to nucleobase intermolecular interactions

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Table S1 Experimental details (pressure transmitting media – paraffine). For all structures: $Na^{2+}\cdot C_5H_3N_5O^{2-}\cdot 7(H_2O)$. M_r = 321.21, monoclinic, $P2_1/c$, Z = 4. Experiments were carried out at 293 K with Mo $K\alpha$ radiation using an *Oxford Diffraction Gemini R Ultra* diffractometer.

	0.2 GPa	0.7 GPa	1.3 GPa	1.9 GPa	2.4 GPa
Crystal data					
a, *b*, *c* (Å)	10.5535(8), 11.730(5), 11.2141(9)	10.5585(7), 11.559(5), 11.0943(8)	10.5565(8), 11.381(6), 11.0175(9)	10.5385(7), 11.308(5), 10.9301(8)	10.560(2), 11.167(16), 10.841(3)
β (°)	101.546(7)	101.771(6)	101.825(7)	102.059(6)	101.957(19)
V (Å^3)	1360.2(6)	1325.5(6)	1295.6(7)	1273.7(6)	1251(2)
Data collection					
Θ_{min}, Θ_{max}	1.942, 22.796	1.943, 24.84	1.95, 25.004	1.959, 23.283	1.934, 1.182
No. of reflections	1243	1749	1619	1626	766
Range of *h*, *k*, *l*	*h* = -15→15, *k* = -6→6, *l* = -16→16	*h* = -15→15, *k* = -6→6, *l* = -16→16	*h* = -15→15, *k* = -5→5, *l* = -16→16	*h* = -15→15, *k* = -5→5, *l* = -16→16	h = -15→15, k = -5→5, l = -15→15

Computer program: *CrysAlis PRO* [1]

Table S2. Experimental details (pressure transmitting media: pentane-isopentane). For all structures: $Na^{2+}\cdot C_5H_3N_5O^{2-}\cdot 7(H_2O)$. Mr = 321.21, monoclinic, $P2_1/c$, Z = 4. Experiments were carried out at 293 K with Mo Kα radiation using an Oxford Diffraction Gemini R Ultra diffractometer.

	1 atm	0.6 GPa	1.2 GPa	1.8 GPa	2.0 GPa	2.3 GPa	2.5 GPa
Crystal data							
a, *b*, *c* (Å)	10.5670 (3), 11.7875 (3), 11.2791 (3)	10.5575 (8), 11.580 (7), 11.1164 (8)	10.5380 (7), 11.433 (7), 10.9920 (8)	10.5441 (7), 11.239 (7), 10.8819 (8)	10.5372 (6), 11.191 (6), 10.8339 (7)	10.5398 (6), 11.142 (5), 10.8026 (6)	10.5403 (10), 11.077 (10), 10.7701 (10)
β (°)	101.443 (3)	101.657 (7)	101.824 (6)	101.974 (6)	102.017 (6)	102.027 (5)	101.972 (8)
V (Å^3)	1376.99 (7)	1331.0 (8)	1296.3 (8)	1261.5 (8)	1249.6 (7)	1240.8 (6)	1230.2 (11)
μ (mm^{-1})	0.19	0.20	0.20	0.21	0.21	0.21	0.21
Data collection							
Absorption correction	Analytical *CrysAlis PRO* [42]	Gaussian Absorb-7 [45]	Gaussian Absorb-7 [45]	Gaussian Absorb-7 [45]	Gaussian Absorb-7 [45]	Gaussian Absorb-7 [45]	Gaussian Absorb-7 [45]
Θ_{min}, Θ_{max}	0.974, 0.992	0.387, 0.476	0.388, 0.476	0.388, 0.476	0.388, 0.476	0.383, 0.476	0.387, 0.476
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26578, 4583, 2931	7917, 1046, 739	7660, 1002, 728	7414, 960, 723	7376, 955, 712	7366, 949, 707	5270, 925, 654
R_{int}	0.062	0.090	0.085	0.089	0.085	0.082	0.103
Range of *h*, *k*, *l*	*h* = -15→15, *k* = -17→17, *l* = -16→16	*h* = -12→12, *k* = -5→5, *l* = -13→13	*h* = -12→12, *k* = -5→5, *l* = -13→13	*h* = -12→12, *k* = -4→5, *l* = -13→13	*h* = -12→12, *k* = -4→4, *l* = -13→13	*h* = -12→12, *k* = -4→4, *l* = -13→13	*h* = -12→12, *k* = -4→4, *l* = -12→12
Refinement							
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.116, 1.01	0.078, 0.223, 1.13	0.073, 0.207, 1.10	0.078, 0.220, 1.09	0.075, 0.223, 1.12	0.075, 0.219, 1.09	0.075, 0.218, 1.09

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No. of reflections	4583	1046	1002	960	955	949	925
No. of parameters	237	81	81	81	81	81	81
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, -0.25	0.42, -0.39	0.38, -0.36	0.40, -0.38	0.38, -0.38	0.37, -0.37	0.40, -0.33

Computer programs: CrysAlis PRO [1], SHELXL-2018/3 [2], Mercury [3].

Table S3. Na…O distances (Å)

№	Contact	1 atm	0.6 GPa	1.2 GPa	1.8 GPa	2.0 GPa	2.3 GPa	2.5 GPa
1	Na1…O7^{i}	2.4744 (14)	2.453 (6)	2.437 (5)	2.432 (6)	2.419 (5)	2.416 (5)	2.409 (5)
2	Na1…O2	2.3538 (14)	2.339 (7)	2.319 (6)	2.299 (7)	2.293 (6)	2.285 (7)	2.273 (7)
3	Na1…O3	2.4416 (15)	2.416 (10)	2.404 (9)	2.382 (10)	2.368 (10)	2.360 (10)	2.361 (11)
4	Na1…O4	2.4707 (14)	2.455 (10)	2.453 (9)	2.435 (10)	2.427 (10)	2.427 (10)	2.425 (10)
5	Na1…O8^{ii}	2.3842 (13)	2.365 (8)	2.348 (7)	2.338 (8)	2.333 (7)	2.323 (7)	2.317 (7)
6	Na1…O5	2.5122 (14)	2.464 (14)	2.434 (12)	2.410 (13)	2.407 (13)	2.395 (13)	2.384 (13)
7	Na2…O5	2.5208 (15)	2.481 (5)	2.451 (5)	2.421 (5)	2.408 (5)	2.404 (5)	2.400 (5)
8	Na2…O4	2.4025 (13)	2.389 (7)	2.363 (6)	2.355 (7)	2.353 (6)	2.345 (7)	2.340 (7)
9	Na2…O7	2.3726 (14)	2.364 (14)	2.337 (13)	2.303 (14)	2.296 (13)	2.305 (14)	2.317 (15)
10	Na2…O6^{iii}	2.4834 (15)	2.489 (7)	2.481 (6)	2.482 (7)	2.475 (7)	2.478 (7)	2.478 (7)
11	Na2…O6	2.3582 (14)	2.364 (6)	2.354 (5)	2.344 (5)	2.342 (5)	2.340 (5)	2.341 (5)
12	Na2…O8	2.4296 (14)	2.423 (14)	2.408 (13)	2.377 (14)	2.369 (14)	2.379 (14)	2.370 (14)

Symmetry code(s): (i) *x*, -*y*+1/2, *z*-1/2; (ii) -*x*, *y*+1/2, -*z*+1/2; (iii) -*x*, -*y*, -*z*+1.

Table S4. Selected angles (º)

Capture	Angle	1 atm	0.6 GPa	1.2 GPa	1.8 GPa	2.0 GPa	2.3 GPa	2.5 GPa
α 1	Na1…O4…Na2	89.45 (5)	87.8 (2)	87.0 (2)	86.1 (2)	85.8 (2)	85.7 (2)	85.7 (2)
α 2	Na1…O5…Na2	85.91 (4)	85.6 (3)	85.5 (3)	85.2 (3)	85.1 (3)	85.2 (3)	85.3 (3)
α 3	Na1^{iii}…O8…Na2	105.72 (5)	104.1 (3)	103.2 (3)	101.8 (3)	101.5 (3)	100.6 (3)	99.9 (3)
α 4	Na2…O7…Na1^{ii}	118.61 (6)	118.6 (5)	119.2 (4)	120.2 (5)	120.9 (5)	120.7 (5)	120.7 (5)
α 5	Na2…O6…Na2^{i}	90.31 (5)	88.1 (2)	86.96 (18)	85.3 (2)	84.83 (19)	84.27 (19)	83.5 (2)
α 6	O6…Na2…O6^{i}	89.69 (5)	91.9 (2)	93.04 (18)	94.7 (2)	95.17 (19)	95.73 (19)	96.5 (2)

Symmetry code(s): (i) *x*, -*y*+1/2, *z*-1/2; (ii) -*x*, *y*+1/2, -*z*+1/2; (iii) -*x*, -*y*, -*z*+1.

Table S5. Distances between non-hydrogen atoms *vs* pressure (The numbering of hydrogen bonds is the same as in Figure 1)

№	*D*—H···*A*	1 atm	0.6 GPa	1.2 GPa	1.8 GPa	2 GPa	2.3 GPa	2.5 GPa
1	O4—H8···N1^{iv}	2.8199 (18)	2.796 (12)	2.753 (11)	2.752 (11)	2.735 (11)	2.742 (11)	2.726 (11)
2	O4—H9···N4	3.0037 (19)	2.959 (10)	2.941 (10)	2.907 (11)	2.894 (10)	2.903 (10)	2.900 (11)
3	O5—H10···O1^{iv}	2.7723 (17)	2.722 (13)	2.719 (12)	2.702 (14)	2.683 (13)	2.678 (13)	2.674 (13)
4	O5—H11···O1^{v}	2.8072 (17)	2.770 (7)	2.741 (6)	2.727 (7)	2.721 (6)	2.716 (6)	2.716 (7)
5	O7—H14···O1^{vi}	2.7930 (17)	2.801 (13)	2.791 (11)	2.795 (13)	2.804 (12)	2.800 (12)	2.784 (12)
6	O6—H13···N3^{vi}	2.9159 (19)	2.871 (15)	2.885 (14)	2.876 (16)	2.875 (15)	2.866 (15)	2.860 (16)
7	O6—H12···O2^{i}	2.819 (2)	2.799 (16)	2.750 (15)	2.744 (16)	2.738 (16)	2.752 (16)	2.751 (17)
8	O8—H17···N3^{vii}	2.8081 (19)	2.773 (8)	2.752 (7)	2.744 (8)	2.737 (8)	2.733 (7)	2.726 (8)
9	O8—H16···O1^{iv}	2.8542 (17)	2.821 (7)	2.798 (6)	2.769 (7)	2.757 (7)	2.752 (7)	2.745 (7)
10	O2—H4···N4^{iii}	2.8006 (19)	2.764 (8)	2.745 (7)	2.722 (8)	2.709 (8)	2.708 (8)	2.698 (8)
11	O3—H6···O5^{ii}	2.9637 (19)	2.920 (14)	2.874 (13)	2.829 (14)	2.824 (13)	2.828 (14)	2.812 (14)
12	O7—H15···O3	2.7773 (19)	2.736 (13)	2.739 (12)	2.732 (13)	2.726 (12)	2.703 (13)	2.699 (13)
13	O3—H7···N2	2.8021 (18)	2.797 (8)	2.788 (7)	2.779 (7)	2.775 (7)	2.774 (7)	2.774 (7)
14	O2—H5···N2	2.983 (2)	2.948 (9)	2.914 (8)	2.882 (9)	2.869 (9)	2.863 (9)	2.862 (9)

Symmetry code(s): (i) -*x*, *y*-1/2, -*z*+1/2; (ii) -*x*, *y*+1/2, -*z*+1/2; (iii) *x*, -*y*+1/2, *z*-1/2; (iv) -*x*+1, *y*-1/2, -*z*+1/2; (v) *x*-1, -*y*+1/2, *z*-1/2; (vi) *x*-1, *y*, *z*; (vii) -*x*+1, -*y*, -*z*+1.

References:

1- Rigaku-Oxford Diffraction Ltd, *CrysAlisPRO*, Yarnton, Oxfordshire, England, 2016.

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3- C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. Van De Streek and P. A. Wood, *J. Appl. Crystallogr.*, 2008, **41**, 466–470.

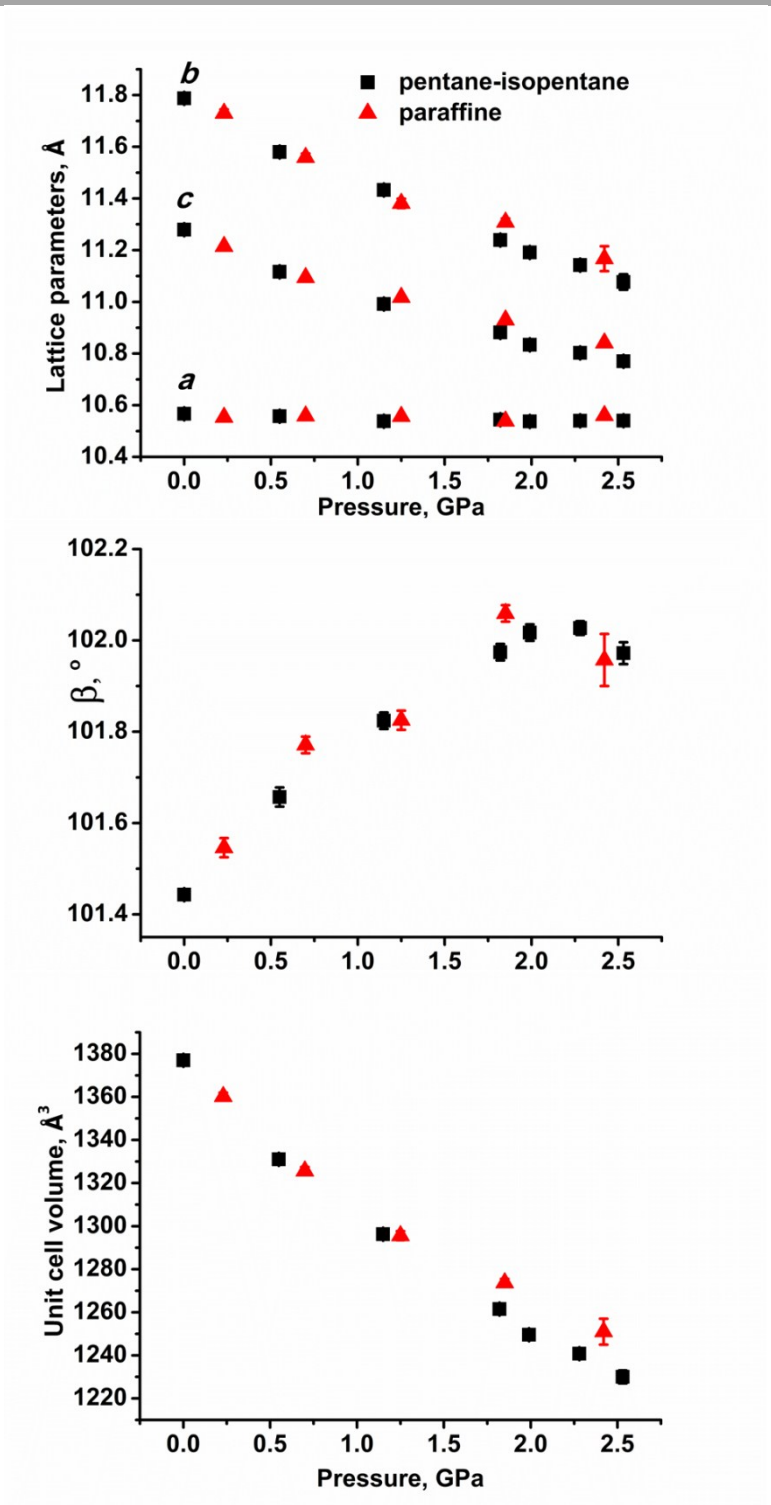

Figure S1. Lattice parameters and volume *vs.* pressure