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Supporting information for article:

A high-pressure single-crystal X-ray diffraction study of potassium guaninate hydrate, $K^{+}\cdot C5H4N5O^{-}\cdot H2O$

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Supplementary Information

Table S1. The compressibility tensor coefficients for $K^+ \cdot C_5H_4N_5O^- \cdot H_2O$

P (GPa)	0.0001	0.2	1.3	3.2
β_{11} (GPa^{-1}, multiplied by 10^3)	-1.1(1)	-1.0(1)	-0.9(9)	-0.6(6)
β_{22} (GPa^{-1}, multiplied by 10^3)	30(3)	30(3)	31(3)	33(3)
β_{33} (GPa^{-1}, multiplied by 10^3)	10(1)	10(1)	10(1)	10(1)
μ_{a1} (°)	71.5	71.5	71.4	71.1
μ_{b2} (°)	0	0	0	0
μ_{c3} (°)	32.1	32.2	32.6	33.3
β_a (GPa^{-1}, multiplied by 10^3)	9(1)	9(1)	9(1)	9(1)
β_b (GPa^{-1}, multiplied by 10^3)	30(2)	30(2)	31(3)	33(3)
β_c (GPa^{-1}, multiplied by 10^3)	7(1)	7(1)	7(1)	7 (1)
β_β (GPa^{-1}, multiplied by 10^3)	3.8(7)	3.8(7)	3.8(7)	3.8(7)
β_V (GPa^{-1}, multiplied by 10^3)	39(4)	40(4)	41(4)	43(4)

Table S2. Shift components of the compressibility tensor for $K^+ \cdot C_5H_4N_5O^- \cdot H_2O$

P (GPa)	0.0001	0.2	1.3	3.2
$\beta_{11(sh)}$ (GPa^{-1}, multiplied by 10^3)	2	2	2	2
$\beta_{33(sh)}$ (GPa^{-1}, multiplied by 10^3)	-9.0	-9.0	-8.9	-8.7
$\mu_{c3\,(sh)}$ (°)	64.7	64.7	64.4	63.9

The orientation of the axes of the compressibility tensor for monoclinic crystals is defined as follows: β_{22} axis is along the *b* axis, two other axes are determined by angles μ_{a1}, μ_{c3}. (for example, μ_{c3} = angle between *c* axis and α_{33}). The coefficients β_a, β_b, β_c correspond to the values of compressibility coefficients along the crystallographic axes *a*, *b*, *c*, respectively; β_β - corresponds to the value of compressibility coefficients of angle β; β_V - corresponds to the value of bulk compressibility coefficient.

Table S3. Distances between non-hydrogen atoms in H-bonds *vs* pressure in $K^+ \cdot C_5H_4N_5O^- \cdot H_2O$ from a laboratory X-ray diffraction experiment. Numbering of atoms and hydrogen bonds corresponds to numbering in Figure 1 in the main text.

№	Pressure (GPa)	0.2	1.3	3.2	1.4 GPa (pressure release)
1	O2W—H5···N9A	2.833 (10)	2.804 (10)	2.806 (9)	2.804 (10)
2	N7A—H2···O3W	2.828 (7)	2.807 (7)	2.743 (7)	2.791 (8)
3	O3W—H11···N7B	2.797 (7)	2.766 (7)	2.724 (7)	2.761 (7)
4	N2A—H3···N3B^{i}	3.028 (8)	2.974 (8)	2.900 (7)	2.962 (8)
5	N1B—H8···O1A^{ii}	2.962 (16)	2.946 (16)	2.877 (16)	2.915 (17)
6	O3W—H12···N7B^{iii}	2.924 (7)	2.872 (7)	2.814 (7)	2.884 (8)

Symmetry codes: (i) *x*+1/2, -*y*+1/2, *z*+1/2; (ii) -*x*+1/2, -*y*+3/2, -*z*+1; (iii) *x*, *y*-1, *z*.

Table S4. Distances between non-hydrogen atoms in H-bonds *vs* pressure in $K^+ \cdot C_5H_4N_5O^- \cdot H_2O$ from a synchrotron experiment. Numbering of atoms and hydrogen bonds corresponds to numbering in Figure 1 in the main text.

№	Pressure (GPa)	0.6	1.3	2.1	2.9
1	O2W—H5···N9A	2.84 (2)	2.83 (2)	2.81 (2)	2.80 (3)
2	N7A—H2···O3W	2.83 (3)	2.81 (3)	2.83 (3)	2.81 (3)
3	O3W—H11···N7B	2.760 (18)	2.751 (19)	2.729 (18)	2.74 (2)
4	N2A—H3···N3B^{i}	3.03 (2)	2.98 (3)	2.94 (2)	2.90 (3)
5	N1B—H8···O1A^{ii}	2.993 (14)	2.958 (15)	2.935 (14)	2.909 (16)
6	O3W—H12···N7B^{iii}	2.897 (18)	2.877 (19)	2.824 (18)	2.82 (2)

№	Pressure (GPa)	3.9	4.9
1	O2W—H5···N9A	2.81 (3)	2.89 (5)
2	N7A—H2···O3W	2.77 (3)	2.93 (6)
3	O3W—H11···N7B	2.74 (2)	2.72 (3)
4	N2A—H3···N3B^{i}	2.88 (3)	2.86 (4)
5	N1B—H8···O1A^{ii}	2.909 (17)	2.86 (3)
6	O3W—H12···N7B^{iii}	2.81 (2)	2.73 (3)

Symmetry codes: (i) *x*+1/2, -*y*+1/2, *z*+1/2; (ii) -*x*+1/2, -*y*+3/2, -*z*+1; (iii) *x*, *y*-1, *z*.

Table S5. Distances between non-hydrogen atoms in H-bonds *vs* pressure in $2Na^{+}•C_5H_3N_5O^{2-}•7H_2O$. Numbering of atoms and hydrogen bonds corresponds to numbering in Figure 1 in the main text. Data were published in: DOI: 10.1039/c9ce00476a

№	Pressure (GPa)	0.0001	0.6	1.2	1.8	2	2.3	2.5
1	O2w—H5···N3	2.983 (2)	2.948 (9)	2.914 (8)	2.882 (9)	2.869 (9)	2.863 (9)	2.862 (9)
2	O3w—H7···N3	2.8021 (18)	2.797 (8)	2.788 (7)	2.779 (7)	2.775 (7)	2.774 (7)	2.774 (7)
3	O4w—H9···N9	3.0037 (19)	2.959 (10)	2.941 (10)	2.907 (11)	2.894 (10)	2.903 (10)	2.900 (11)
4	O7w—H15···O3w	2.7773 (19)	2.736 (13)	2.739 (12)	2.732 (13)	2.726 (12)	2.703 (13)	2.699 (13)
5	O6w—H12···O2w^{i}	2.819 (2)	2.799 (16)	2.750 (15)	2.744 (16)	2.738 (16)	2.752 (16)	2.751 (17)
6	O3w—H6···O5w^{ii}	2.9637 (19)	2.920 (14)	2.874 (13)	2.829 (14)	2.824 (13)	2.828 (14)	2.812 (14)
7	O2w—H4···N9^{iii}	2.8006 (19)	2.764 (8)	2.745 (7)	2.722 (8)	2.709 (8)	2.708 (8)	2.698 (8)
8	O4w—H8···N1^{iv}	2.8199 (18)	2.796 (12)	2.753 (11)	2.752 (11)	2.735 (11)	2.742 (11)	2.726 (11)
9	O5w—H10···O1^{iv}	2.7723 (17)	2.722 (13)	2.719 (12)	2.702 S(14)	2.683 (13)	2.678 (13)	2.674 (13)
10	O8w—H16···O1^{iv}	2.8542 (17)	2.821 (7)	2.798 (6)	2.769 (7)	2.757 (7)	2.752 (7)	2.745 (7)

11	O5w—H11···O1^{v}	2.8072 (17)	2.770 (7)	2.741 (6)	2.727 (7)	2.721 (6)	2.716 (6)	2.716 (7)
12	O6w—H13···N7^{vi}	2.9159 (19)	2.871 (15)	2.885 (14)	2.876 (16)	2.875 (15)	2.866 (15)	2.860 (16)
13	O7w—H14···O1^{vi}	2.7930 (17)	2.801 (13)	2.791 (11)	2.795 (13)	2.804 (12)	2.800 (12)	2.784 (12)
14	O8w—H17···N7^{vii}	2.8081 (19)	2.773 (8)	2.752 (7)	2.744 (8)	2.737 (8)	2.733 (7)	2.726 (8)

Symmetry codes: (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.

Table S6. Distances between non-hydrogen atoms in H-bonds *vs* temperature in $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$ (variable temperature). Numbering of hydrogen bonds corresponds to numbering in Figure 1 in the main text. Data were published in https://doi.org/10.1107/S205252062100754X

№	Temperature (K)	100	150	200	250	300
1	O2W—H5···N9A	2.810 (2)	2.814 (2)	2.8162 (19)	2.8179 (19)	2.825 (2)
2	N7A—H2···O3W	2.820 (2)	2.822 (2)	2.8254 (18)	2.8285 (19)	2.835 (2)
3	O3W—H11···N7B	2.7718 (19)	2.775 (2)	2.7734 (18)	2.7793 (19)	2.782 (2)
4	N2A—H3···N3B^{i}	3.019 (2)	3.026 (2)	3.0376 (19)	3.044 (2)	3.055 (2)
5	N1B—H8···O1A^{ii}	2.967 (2)	2.972 (2)	2.9793 (18)	2.9893 (18)	2.9957 (19)
6	O3W—H12···N7B^{iii}	2.907 (2)	2.914 (2)	2.9175 (19)	2.925 (2)	2.935 (2)

Table S7. Distances between non-hydrogen atoms vs temperature in $2Na^{+}\cdot C_5H_3N_5O^{2-}\cdot\cdot 7H_2O$. Numbering of atoms and hydrogen bonds corresponds to numbering in Figure 1 in the main text. Data were published in https://doi.org/10.1107/S205252062100754X

№	Temperature (K)	100	125	150	175
1	O2W—H5···N3	2.9521 (15)	2.9544 (14)	2.9566 (15)	2.9601 (16)
2	O3W—H7···N3	2.7971 (13)	2.7973 (13)	2.7985 (13)	2.7988 (14)
3	O4W—H9···N9	2.9814 (14)	2.9811 (14)	2.9848 (14)	2.9889 (15)
4	O7W—H15···O3W	2.7539 (12)	2.7540 (12)	2.7551 (12)	2.7583 (13)
5	O6W—H12···O2W^{i}	2.7890 (13)	2.7911 (12)	2.7945 (13)	2.7949 (14)
6	O3W—H6···O5W^{ii}	2.9149 (12)	2.9186 (12)	2.9218 (12)	2.9268 (13)
7	O2W—H4···N9^{iii}	2.7806 (13)	2.7799 (13)	2.7817 (13)	2.7841 (14)
8	O4W—H8···N1^{iv}	2.8034 (13)	2.8044 (13)	2.8034 (13)	2.8049 (14)
9	O5W—H10···O1^{iv}	2.7551 (12)	2.7566 (11)	2.7570 (11)	2.7587 (12)
10	O8W— H16···O1^{iv}	2.8271 (12)	2.8291 (12)	2.8307 (12)	2.8335 (13)
11	O5W—H11···O1^{v}	2.7770 (13)	2.7791 (13)	2.7808 (13)	2.7828 (14)
12	O6W—H13···N7^{vi}	2.9081 (13)	2.9078 (13)	2.9075 (13)	2.9079 (14)
13	O7W—H14···O1^{vi}	2.7815 (12)	2.7827 (12)	2.7827 (12)	2.7840 (13)
14	O8W— H17···N7^{vii}	2.7853 (14)	2.7876 (14)	2.7888 (14)	2.7919 (15)

№	Temperature (K)	200	225	250	275
1	O2W—H5···N3	2.9608 (16)	2.9690 (16)	2.9703 (17)	2.9757 (19)
2	O3W—H7···N3	2.7972 (14)	2.7974 (14)	2.7973 (15)	2.7970 (16)
3	O4W—H9···N9	2.9908 (15)	2.9925 (15)	2.9977 (16)	2.9994 (18)
4	O7W—H15···O3W	2.7604 (13)	2.7632 (13)	2.7671 (14)	2.7718 (16)
5	O6W—H12···O2W^{i}	2.7995 (14)	2.8026 (14)	2.8074 (16)	2.8118 (17)
6	O3W—H6···O5W^{ii}	2.9334 (13)	2.9410 (13)	2.9494 (14)	2.9585 (16)
7	O2W—H4···N9^{iii}	2.7859 (14)	2.7885 (14)	2.7922 (15)	2.7941 (17)
8	O4W—H8···N1^{iv}	2.8067 (14)	2.8098 (14)	2.8115 (15)	2.8137 (16)
9	O5W—H10···O1^{iv}	2.7606 (12)	2.7613 (12)	2.7621 (13)	2.7652 (15)
10	O8W—H16···O1^{iv}	2.8345 (13)	2.8401 (13)	2.8407 (14)	2.8456 (16)
11	O5W—H11···O1^{v}	2.7899 (14)	2.7921 (14)	2.7962 (15)	2.8007 (16)
12	O6W—H13···N7^{vi}	2.9087 (14)	2.9098 (14)	2.9102 (15)	2.9120 (17)
13	O7W—H14···O1^{vi}	2.7847 (13)	2.7857 (13)	2.7884 (14)	2.7869 (15)
14	O8W—H17···N7^{vii}	2.7944 (15)	2.7953 (15)	2.7990 (16)	2.8010 (17)

№	Temperature (K)	298
1	O2W—H5···N3	2.9789 (17)
2	O3W—H7···N3	2.7974 (15)
3	O4W—H9···N9	3.0031 (16)
4	O7W—H15···O3W	2.7736 (15)
5	O6W—H12···O2W^{i}	2.8184 (16)
6	O3W—H6···O5W^{ii}	2.9699 (15)
7	O2W—H4···N9^{iii}	2.7981 (16)
8	O4W—H8···N1^{iv}	2.8148 (15)
9	O5W—H10···O1^{iv}	2.7671 (14)
10	O8W—H16···O1^{iv}	2.8504 (14)
11	O5W—H11···O1^{v}	2.8073 (15)
12	O6W—H13···N7^{vi}	2.9114 (16)
13	O7W— H14···O1^{vi}	2.7896 (14)
14	O8W—H17···N7^{vii}	2.8028 (16)

Symmetry codes: (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.

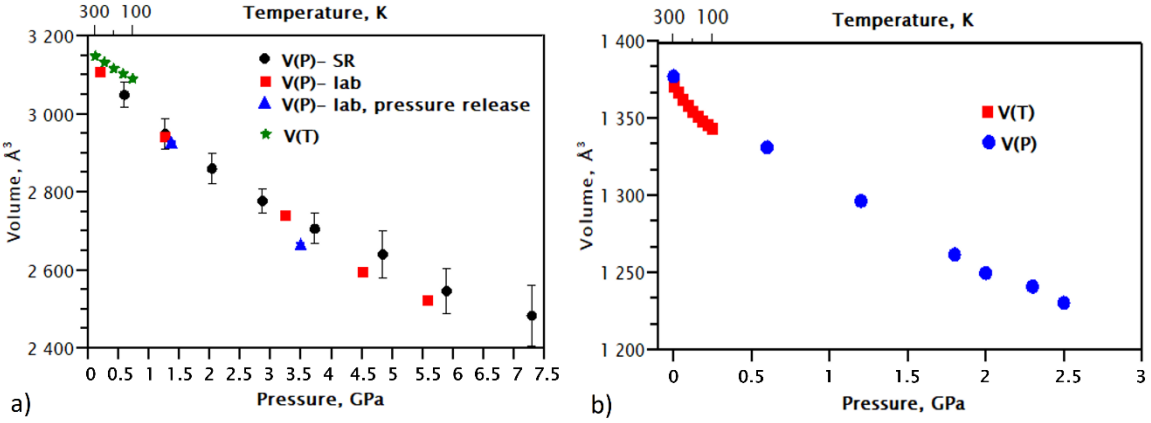

Figure S1. a) Changes in the unit cell volume of $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$ on cooling and on hydrostatic compression; b) Changes in the unit cell volume of $2Na^{+}\cdot C_5H_3N_5O_2{-}\cdot 7H_2O$ on cooling and on hydrostatic compression

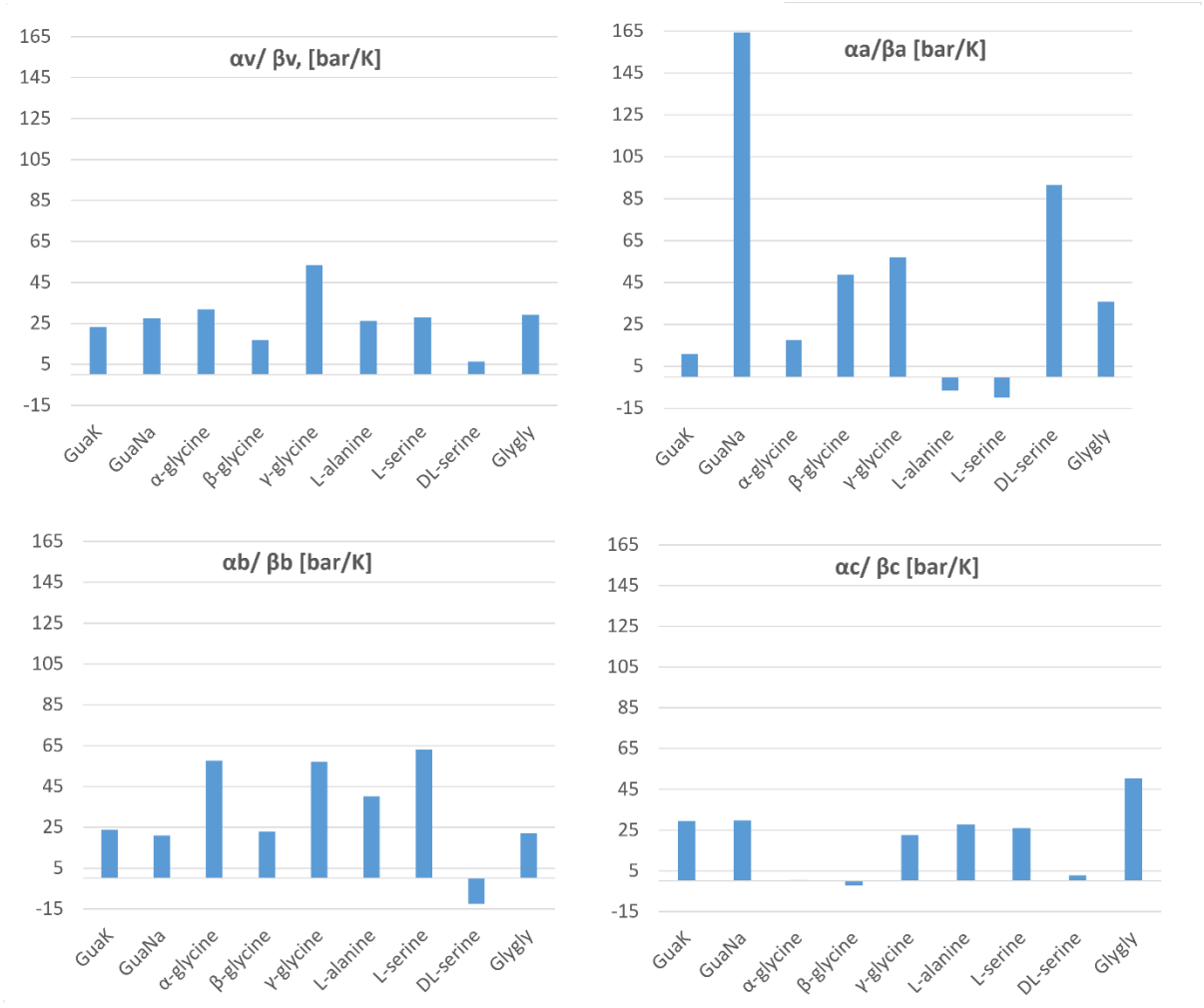

Figure S2 Baric equivalents of thermal strain for the salt hydrates of guanine compared with those for selected amino acids