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Supporting information for article:

A new guaninate hydrate $K^{+}\cdot C5H4N5O^{-}\cdot H2O$: crystal structure from 100 to 300 K in a comparison with $2Na^{+}\cdot C5H3N5O^{2-}\cdot 7H2O$

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SUPPLEMENTARY INFORMATION

1. Crystallization

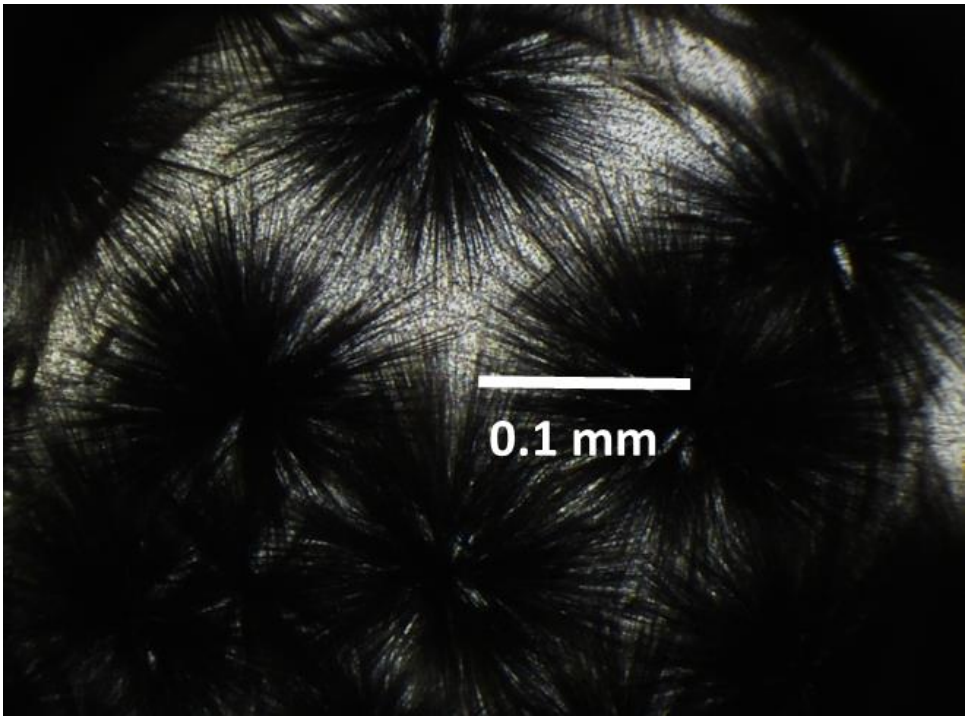

Figure S1. The crystals of $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$ growing as the ball-shaped spherulites, which transformed later into the spherical aggregates of needles.

2. Coordination of metal cations and geometries of hydrogen bonds

Table S1. Hydrogen-bond parameters for $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
100 K				
O2W—H5···N9A	0.835 (16)	1.997 (17)	2.810 (2)	164 (2)
N7A—H2···O3W	0.87 (2)	1.96 (2)	2.820 (2)	173 (2)
O3W—H11···N7B	0.963 (13)	1.825 (15)	2.7718 (19)	167.1 (18)

N2A—H3···N3B^{i}	0.89 (2)	2.19 (2)	3.019 (2)	155.5 (19)
N1B—H8···O1A^{ii}	0.84 (2)	2.13 (2)	2.967 (2)	173.1 (19)
O3W—H12···N7B^{iii}	0.947 (13)	1.992 (16)	2.907 (2)	161.8 (18)
150 K				
O2W—H5···N9A	0.812 (17)	2.021 (18)	2.814 (2)	165 (2)
N7A—H2···O3W	0.84 (2)	1.98 (2)	2.822 (2)	174 (2)
O3W—H11···N7B	0.935 (13)	1.862 (16)	2.775 (2)	165 (2)
N2A—H3···N3B^{i}	0.90 (2)	2.20 (2)	3.026 (2)	153.1 (19)
N1B—H8···O1A^{ii}	0.85 (2)	2.13 (2)	2.972 (2)	172.9 (19)
O3W—H12···N7B^{iii}	0.922 (13)	2.034 (17)	2.914 (2)	158.9 (19)
200 K				
O2W—H5···N9A	0.802 (15)	2.037 (16)	2.8162 (19)	163.6 (19)
N7A—H2···O3W	0.864 (19)	1.965 (19)	2.8254 (18)	173.3 (19)
O3W—H11···N7B	0.943 (12)	1.848 (14)	2.7734 (18)	166.6 (18)
N2A—	0.867 (19)	2.224 (19)	3.0376 (19)	156.1 (17)

H3···N3B^{i}				
N1B—H8···O1A^{ii}	0.824 (18)	2.158 (19)	2.9793 (18)	174.1 (16)
O3W—H12···N7B^{iii}	0.931 (12)	2.026 (15)	2.9175 (19)	159.9 (16)
250 K				
O2W—H5···N9A	0.811 (15)	2.024 (16)	2.8179 (19)	166 (2)
N7A—H2···O3W	0.871 (19)	1.962 (19)	2.8285 (19)	172.6 (19)
O3W—H11···N7B	0.945 (12)	1.855 (14)	2.7793 (19)	165.4 (19)
N2A—H3···N3B^{i}	0.862 (19)	2.242 (19)	3.044 (2)	154.8 (17)
N1B—H8···O1A^{ii}	0.840 (18)	2.155 (19)	2.9893 (18)	172.1 (16)
O3W—H12···N7B^{iii}	0.933 (13)	2.034 (15)	2.925 (2)	159.1 (17)
300 K				
O2W—H5···N9A	0.819 (16)	2.031 (17)	2.825 (2)	163 (2)
N7A—H2···O3W	0.86 (2)	1.97 (2)	2.835 (2)	173 (2)
O3W—H11···N7B	0.938 (13)	1.861 (15)	2.782 (2)	166.7 (19)
N2A—H3···N3B^{i}	0.86 (2)	2.26 (2)	3.055 (2)	153.6 (18)

N1B—H8···O1A^{ii}	0.821 (19)	2.181 (19)	2.9957 (19)	171.7 (17)
O3W—H12···N7B^{iii}	0.925 (13)	2.060 (16)	2.935 (2)	157.4 (18)

Symmetry code(s): (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 S2. Selected hydrogen-bond parameters for sodium salt of guanine

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
100 K				
O2W—H5···N3	0.852 (19)	2.115 (19)	2.9521 (15)	167.2 (16)
O3W—H7···N3	0.836 (18)	1.978 (18)	2.7971 (13)	166.2 (16)
O4W—H9···N9	0.802 (19)	2.180 (19)	2.9814 (14)	175.8 (17)
O7W—H15···O3W	0.808 (18)	1.956 (18)	2.7539 (12)	169.6 (17)
O6W—H12···O2W^{i}	0.818 (18)	1.979 (19)	2.7890 (13)	170.3 (17)
O3W—H6···O5W^{ii}	0.809 (18)	2.132 (18)	2.9149 (12)	162.9 (16)
O2W—H4···N9^{iii}	0.785 (18)	2.001 (18)	2.7806 (13)	172.1 (17)
O4W—H8···N1^{iv}	0.813 (18)	1.994 (18)	2.8034 (13)	173.6 (17)
O5W—H10···O1^{iv}	0.826 (18)	1.938 (18)	2.7551 (12)	169.9 (16)
O8W—	0.807 (18)	2.030 (18)	2.8271 (12)	169.5 (16)

H16···O1^{iv}				
O5W—H11···O1^{v}	0.814 (18)	1.976 (19)	2.7770 (13)	167.8 (16)
O6W—H13···N7^{vi}	0.845 (18)	2.072 (18)	2.9081 (13)	170.2 (16)
O7W—H14···O1^{vi}	0.839 (18)	1.974 (18)	2.7815 (12)	161.2 (16)
O8W—H17···N7^{vii}	0.836 (18)	1.956 (18)	2.7853 (14)	171.4 (16)
125 K				
O2W—H5···N3	0.850 (18)	2.117 (18)	2.9544 (14)	168.4 (15)
O3W—H7···N3	0.830 (17)	1.990 (17)	2.7973 (13)	164.0 (16)
O4W—H9···N9	0.805 (18)	2.177 (18)	2.9811 (14)	176.7 (16)
O7W—H15···O3W	0.825 (17)	1.937 (17)	2.7540 (12)	170.1 (16)
O6W—H12···O2W^{i}	0.800 (18)	2.000 (18)	2.7911 (12)	170.1 (16)
O3W—H6···O5W^{ii}	0.821 (17)	2.121 (17)	2.9186 (12)	163.6 (15)
O2W—H4···N9^{iii}	0.794 (17)	1.990 (18)	2.7799 (13)	173.0 (16)
O4W—H8···N1^{iv}	0.807 (17)	2.000 (17)	2.8044 (13)	175.2 (16)
O5W—H10···O1^{iv}	0.840 (17)	1.925 (17)	2.7566 (11)	170.1 (15)
O8W—H16···O1^{iv}	0.783 (17)	2.056 (18)	2.8291 (12)	169.1 (16)

O5W—H11···O1^{v}	0.818 (17)	1.970 (18)	2.7791 (13)	170.1 (16)
O6W—H13···N7^{vi}	0.851 (17)	2.065 (17)	2.9078 (13)	171.0 (15)
O7W—H14···O1^{vi}	0.825 (17)	1.991 (17)	2.7827 (12)	160.6 (15)
O8W—H17···N7^{vii}	0.831 (17)	1.961 (18)	2.7876 (14)	172.7 (15)
150 K				
O2W—H5···N3	0.855 (19)	2.115 (19)	2.9566 (15)	168.0 (16)
O3W—H7···N3	0.823 (18)	1.997 (18)	2.7985 (13)	164.3 (16)
O4W—H9···N9	0.792 (18)	2.194 (18)	2.9848 (14)	176.2 (17)
O7W—H15···O3W	0.826 (17)	1.940 (18)	2.7551 (12)	169.2 (17)
O6W—H12···O2W^{i}	0.789 (18)	2.013 (19)	2.7945 (13)	170.6 (17)
O3W—H6···O5W^{ii}	0.817 (17)	2.127 (18)	2.9218 (12)	164.3 (16)
O2W—H4···N9^{iii}	0.799 (18)	1.988 (18)	2.7817 (13)	172.1 (16)
O4W—H8···N1^{iv}	0.827 (17)	1.980 (17)	2.8034 (13)	173.9 (16)
O5W—H10···O1^{iv}	0.839 (17)	1.926 (18)	2.7570 (11)	170.4 (16)
O8W—H16···O1^{iv}	0.820 (18)	2.021 (18)	2.8307 (12)	169.1 (16)
O5W—	0.789 (18)	2.003 (18)	2.7808 (13)	168.6 (17)

H11···O1^{v}				
O6W—H13···N7^{vi}	0.864 (18)	2.053 (18)	2.9075 (13)	170.0 (16)
O7W—H14···O1^{vi}	0.832 (18)	1.985 (18)	2.7827 (12)	160.3 (16)
O8W—H17···N7^{vii}	0.828 (18)	1.966 (18)	2.7888 (14)	172.0 (16)
175 K				
O2W—H5···N3	0.88 (2)	2.10 (2)	2.9601 (16)	168.5 (17)
O3W—H7···N3	0.835 (19)	1.982 (19)	2.7988 (14)	165.9 (17)
O4W—H9···N9	0.794 (19)	2.20 (2)	2.9889 (15)	176.1 (18)
O7W—H15···O3W	0.809 (19)	1.958 (19)	2.7583 (13)	170.2 (18)
O6W—H12···O2W^{i}	0.82 (2)	1.98 (2)	2.7949 (14)	170.0 (18)
O3W—H6···O5W^{ii}	0.806 (19)	2.148 (19)	2.9268 (13)	162.5 (17)
O2W—H4···N9^{iii}	0.77 (2)	2.02 (2)	2.7841 (14)	171.9 (18)
O4W—H8···N1^{iv}	0.818 (19)	1.991 (19)	2.8049 (14)	173.2 (17)
O5W—H10···O1^{iv}	0.831 (18)	1.938 (19)	2.7587 (12)	169.1 (17)
O8W—H16···O1^{iv}	0.804 (19)	2.042 (19)	2.8335 (13)	168.0 (17)
O5W—H11···O1^{v}	0.815 (19)	1.98 (2)	2.7828 (14)	169.2 (17)

O6W—H13···N7^{vi}	0.847 (19)	2.067 (19)	2.9079 (14)	172.0 (17)
O7W—H14···O1^{vi}	0.828 (19)	1.989 (19)	2.7840 (13)	160.9 (17)
O8W—H17···N7^{vii}	0.840 (19)	1.957 (19)	2.7919 (15)	172.3 (17)
200 K				
O2W—H5···N3	0.89 (2)	2.09 (2)	2.9608 (16)	167.8 (17)
O3W—H7···N3	0.819 (19)	2.001 (19)	2.7972 (14)	164.1 (18)
O4W—H9···N9	0.791 (19)	2.20 (2)	2.9908 (15)	175.3 (18)
O7W—H15···O3W	0.809 (19)	1.962 (19)	2.7604 (13)	169.0 (18)
O6W—H12···O2W^{i}	0.81 (2)	2.00 (2)	2.7995 (14)	170.7 (18)
O3W—H6···O5W^{ii}	0.821 (19)	2.140 (19)	2.9334 (13)	162.5 (17)
O2W—H4···N9^{iii}	0.776 (19)	2.02 (2)	2.7859 (14)	170.6 (18)
O4W—H8···N1^{iv}	0.825 (18)	1.983 (19)	2.8067 (14)	175.2 (17)
O5W—H10···O1^{iv}	0.830 (19)	1.938 (19)	2.7606 (12)	170.9 (17)
O8W—H16···O1^{iv}	0.816 (19)	2.033 (19)	2.8345 (13)	167.1 (17)
O5W—H11···O1^{v}	0.786 (19)	2.01 (2)	2.7899 (14)	169.4 (18)
O6W—	0.849 (19)	2.067 (19)	2.9087 (14)	171.2 (17)

H13···N7^{vi}				
O7W—H14···O1^{vi}	0.833 (19)	1.982 (19)	2.7847 (13)	161.3 (17)
O8W—H17···N7^{vii}	0.819 (19)	1.980 (19)	2.7944 (15)	172.4 (17)
225 K				
O2W—H5···N3	0.86 (2)	2.12 (2)	2.9690 (16)	167.5 (17)
O3W—H7···N3	0.840 (19)	1.984 (19)	2.7974 (14)	163.0 (17)
O4W—H9···N9	0.801 (19)	2.194 (19)	2.9925 (15)	175.1 (17)
O7W—H15···O3W	0.802 (18)	1.973 (19)	2.7632 (13)	168.3 (18)
O6W—H12···O2W^{i}	0.81 (2)	2.00 (2)	2.8026 (14)	171.6 (18)
O3W—H6···O5W^{ii}	0.814 (18)	2.159 (19)	2.9410 (13)	161.0 (17)
O2W—H4···N9^{iii}	0.768 (19)	2.028 (19)	2.7885 (14)	170.7 (18)
O4W—H8···N1^{iv}	0.823 (18)	1.989 (18)	2.8098 (14)	175.7 (17)
O5W—H10···O1^{iv}	0.853 (18)	1.917 (18)	2.7613 (12)	170.2 (16)
O8W—H16···O1^{iv}	0.789 (18)	2.063 (19)	2.8401 (13)	168.3 (17)
O5W—H11···O1^{v}	0.779 (19)	2.022 (19)	2.7921 (14)	169.7 (18)
O6W—H13···N7^{vi}	0.854 (19)	2.066 (19)	2.9098 (14)	169.5 (17)

O7W—H14···O1^{vi}	0.844 (19)	1.972 (19)	2.7857 (13)	161.6 (17)
O8W—H17···N7^{vii}	0.838 (18)	1.962 (19)	2.7953 (15)	173.1 (16)
250 K				
O2W—H5···N3	0.87 (2)	2.11 (2)	2.9703 (17)	168.5 (18)
O3W—H7···N3	0.84 (2)	1.98 (2)	2.7973 (15)	162.8 (18)
O4W—H9···N9	0.80 (2)	2.20 (2)	2.9977 (16)	175.4 (18)
O7W—H15···O3W	0.814 (19)	1.96 (2)	2.7671 (14)	169.8 (19)
O6W—H12···O2W^{i}	0.80 (2)	2.01 (2)	2.8074 (16)	171.0 (19)
O3W—H6···O5W^{ii}	0.82 (2)	2.15 (2)	2.9494 (14)	162.1 (17)
O2W—H4···N9^{iii}	0.76 (2)	2.05 (2)	2.7922 (15)	167 (2)
O4W—H8···N1^{iv}	0.826 (19)	1.988 (19)	2.8115 (15)	175.2 (18)
O5W—H10···O1^{iv}	0.823 (19)	1.94 (2)	2.7621 (13)	172.2 (18)
O8W—H16···O1^{iv}	0.82 (2)	2.03 (2)	2.8407 (14)	168.2 (17)
O5W—H11···O1^{v}	0.77 (2)	2.04 (2)	2.7962 (15)	169.7 (19)
O6W—H13···N7^{vi}	0.86 (2)	2.07 (2)	2.9102 (15)	169.4 (18)
O7W—	0.83 (2)	1.99 (2)	2.7884 (14)	160.5 (18)

H14···O1^{vi}				
O8W—H17···N7^{vii}	0.809 (19)	1.99 (2)	2.7990 (16)	172.7 (18)
275 K				
O2W—H5···N3	0.88 (2)	2.12 (2)	2.9757 (19)	166 (2)
O3W—H7···N3	0.87 (2)	1.96 (2)	2.7970 (16)	162 (2)
O4W—H9···N9	0.81 (2)	2.19 (2)	2.9994 (18)	177 (2)
O7W—H15···O3W	0.81 (2)	1.97 (2)	2.7718 (16)	168 (2)
O6W—H12···O2W^{i}	0.82 (2)	2.00 (2)	2.8118 (17)	170 (2)
O3W—H6···O5W^{ii}	0.84 (2)	2.15 (2)	2.9585 (16)	163 (2)
O2W—H4···N9^{iii}	0.80 (2)	2.01 (2)	2.7941 (17)	170 (2)
O4W—H8···N1^{iv}	0.82 (2)	2.00 (2)	2.8137 (16)	174 (2)
O5W—H10···O1^{iv}	0.82 (2)	1.96 (2)	2.7652 (15)	170 (2)
O8W—H16···O1^{iv}	0.82 (2)	2.03 (2)	2.8456 (16)	170.4 (19)
O5W—H11···O1^{v}	0.77 (2)	2.04 (2)	2.8007 (16)	171 (2)
O6W—H13···N7^{vi}	0.86 (2)	2.06 (2)	2.9120 (17)	169 (2)
O7W—H14···O1^{vi}	0.86 (2)	1.96 (2)	2.7869 (15)	159.5 (19)

O8W—H17···N7^{vii}	0.81 (2)	2.00 (2)	2.8010 (17)	172 (2)
298 K				
O2W—H5···N3	0.90 (2)	2.09 (2)	2.9789 (17)	167.5 (17)
O3W—H7···N3	0.84 (2)	1.99 (2)	2.7974 (15)	158.9 (18)
O4W—H9···N9	0.79 (2)	2.22 (2)	3.0031 (16)	177.4 (19)
O7W—H15···O3W	0.81 (2)	1.97 (2)	2.7736 (15)	169.3 (19)
O6W—H12···O2W^{i}	0.81 (2)	2.02 (2)	2.8184 (16)	170.3 (19)
O3W—H6···O5W^{ii}	0.83 (2)	2.17 (2)	2.9699 (15)	161.2 (18)
O2W—H4···N9^{iii}	0.77 (2)	2.04 (2)	2.7981 (16)	169 (2)
O4W—H8···N1^{iv}	0.832 (19)	1.98 (2)	2.8148 (15)	175.9 (18)
O5W—H10···O1^{iv}	0.83 (2)	1.95 (2)	2.7671 (14)	169.9 (18)
O8W—H16···O1^{iv}	0.81 (2)	2.05 (2)	2.8504 (14)	169.4 (17)
O5W—H11···O1^{v}	0.75 (2)	2.07 (2)	2.8073 (15)	170 (2)
O6W—H13···N7^{vi}	0.88 (2)	2.04 (2)	2.9114 (16)	169.1 (17)
O7W—H14···O1^{vi}	0.82 (2)	2.00 (2)	2.7896 (14)	161.7 (18)
O8W—	0.802 (19)	2.01 (2)	2.8028 (16)	171.0 (18)

H17···N7^{vii}				

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.

Table S3. Selected geometric parameters (Å). Distances between metal cations and environment for $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$

Contact	Temperature (K)				
	100(2)	150(2)	200(2)	250(2)	300(2)
K1—N3B^{i}	2.9130 (14)	2.9140 (15)	2.9163 (13)	2.9186 (13)	2.9178 (14)
K1—N3A	2.9012 (16)	2.9036 (17)	2.9063 (14)	2.9093 (15)	2.9110 (16)
K1—N3A^{ii}	3.2339 (15)	3.2421 (16)	3.2518 (14)	3.2646 (14)	3.2771 (15)
K1—N9B^{i}	3.0276 (16)	3.0341 (17)	3.0366 (14)	3.0424 (15)	3.0469 (16)
K1—N9B^{iii}	3.1060 (15)	3.1152 (16)	3.1218 (14)	3.1320 (14)	3.1435 (15)
K1—N9A	3.4640 (16)	3.4627 (18)	3.4621 (16)	3.4582 (17)	3.4567 (18)
O1A—K2	2.6188 (13)	2.6205 (13)	2.6224 (11)	2.6264 (12)	2.6310 (12)
O1A—K2^{iv}	2.6771 (13)	2.6792 (14)	2.6822 (12)	2.6873 (12)	2.6931 (13)
K1—O2W	2.7230 (14)	2.7302 (15)	2.7347 (13)	2.7441 (14)	2.7538 (15)
K1—O2W^{ii}	2.7698 (14)	2.7758 (16)	2.7834 (14)	2.7933 (14)	2.8004 (16)
K1—O2W^{v}	3.0372 (15)	3.0428 (15)	3.0491 (13)	3.0583 (14)	3.0678 (16)
K2—O1B	2.6914 (13)	2.6936 (14)	2.6945 (12)	2.6978 (12)	2.7022 (13)
K2—O1B^{iv}	2.7182 (13)	2.7234 (14)	2.7305 (12)	2.7382 (13)	2.7449 (14)
K2—O1B^{vi}	2.7336 (14)	2.7378 (14)	2.7411 (12)	2.7459 (13)	2.7508 (13)
K2—O3W	2.9130 (15)	2.9218 (17)	2.9329 (15)	2.9443 (16)	2.9559 (18)

Symmetry code(s): (i) *x*+1/2, −*y*+3/2, *z*+1/2; (ii) *x*, *y*+1, *z*; (iii) *x*+1/2, −*y*+1/2, *z*+1/2; (iv) *x*, *y*−1, *z*; (v) −*x*+1, −*y*, −*z*+2; (vi) −*x*+1/2, −*y*+3/2, −*z*+1.

Table S4. Selected geometric parameters (º). Angles between metal cations and environment for $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$

Angle **(º)**	100 K	(150K)	(200K)	250 K	300 K
N3B^{i}—K1—N3A^{ii}	82.02 (4)	82.02 (4)	82.01 (4)	81.93 (4)	81.87 (4)
N3B^{i}—K1—N9B^{i}	47.97 (4)	47.90 (4)	47.88 (4)	47.82 (4)	47.70 (4)
N3B^{i}—K1—N9B^{iii}	69.44 (4)	69.46 (4)	69.51 (4)	69.65 (4)	69.74 (4)
N3B^{i}—K1—N9A	137.40 (4)	137.41 (4)	137.42 (4)	137.43 (4)	137.48 (4)
N3A—K1—N3B^{i}	99.67 (4)	99.73 (5)	99.74 (4)	99.79 (4)	99.86 (4)
N3A—K1—N3A^{ii}	77.00 (4)	77.16 (4)	77.28 (3)	77.39 (3)	77.52 (3)
N3A—K1—N9B^{i}	147.34 (4)	147.34 (5)	147.31 (4)	147.30 (4)	147.25 (4)
N3A—K1—N9B^{iii}	96.94 (4)	96.84 (5)	96.72 (4)	96.67 (4)	96.57 (4)
N3A—K1—N9A	43.82 (4)	43.76 (4)	43.76 (4)	43.73 (4)	43.76 (4)
N3A^{ii}—K1—N9A	70.22 (4)	70.32 (4)	70.41 (4)	70.51 (4)	70.59 (4)
N9B^{i}—K1—N3A^{ii}	91.80 (4)	91.67 (4)	91.51 (4)	91.37 (4)	91.23 (4)
N9B^{iii}—K1—N3A^{ii}	149.52 (4)	149.54 (4)	149.58 (4)	149.64 (4)	149.67 (4)
N9B^{i}—K1—N9B^{iii}	77.22 (3)	77.32 (4)	77.49 (3)	77.61 (3)	77.72 (3)
N9B^{i}—K1—N9A	157.25 (4)	157.28 (5)	157.25 (4)	157.24 (4)	157.20 (4)
N9B^{iii}—K1—N9A	125.26 (4)	125.15 (5)	125.02 (4)	124.91 (4)	124.84 (5)
O2W—K1—O2W^{ii}	88.36 (4)	88.49 (4)	88.62 (4)	88.66 (4)	88.75 (4)
O2W—K1—O2W^{iv}	83.85 (4)	83.91 (4)	83.92 (4)	83.95 (4)	83.95 (4)

O2W^{ii}—K1—O2W^{iv}	63.08 (4)	63.05 (5)	63.05 (4)	63.03 (4)	62.91 (5)
O1B—K2—O1B^{v}	90.09 (4)	90.34 (4)	90.55 (3)	90.77 (4)	90.98 (4)
O1B—K2—O1B^{vi}	85.97 (4)	85.97 (4)	85.97 (4)	86.02 (4)	86.02 (4)
O1B^{v}—K2—O1B^{vi}	81.12 (4)	81.10 (4)	81.09 (4)	81.06 (4)	80.99 (4)
O1B—K2—O3W	107.64 (4)	107.58 (4)	107.52 (4)	107.47 (4)	107.43 (4)
O1B^{v}—K2—O3W	82.92 (4)	82.87 (4)	82.81 (4)	82.76 (4)	82.80 (4)
O1B^{vi}—K2—O3W	159.01 (4)	159.05 (5)	159.07 (4)	159.05 (4)	159.09 (5)
O1A—K2—O1B	169.06 (4)	169.11 (4)	169.18 (4)	169.29 (4)	169.33 (4)
O1A^{ii}—K2—O1B	87.34 (4)	87.08 (4)	86.90 (4)	86.72 (4)	86.51 (4)
O1A—K2—O1B^{v}	87.96 (4)	87.65 (4)	87.36 (4)	87.10 (4)	86.88 (4)
O1A^{ii}—K2—O1B^{v}	169.16 (4)	169.22 (4)	169.32 (4)	169.44 (4)	169.48 (4)
O1A—K2—O1B^{vi}	83.09 (4)	83.15 (4)	83.22 (4)	83.28 (4)	83.32 (4)
O1A^{ii}—K2—O1B^{vi}	88.19 (4)	88.28 (4)	88.38 (4)	88.52 (4)	88.64 (4)
O1A—K2—O1A^{ii}	92.57 (4)	92.92 (4)	93.21 (3)	93.47 (4)	93.71 (4)
O1A—K2—O3W	82.81 (4)	82.79 (4)	82.76 (4)	82.69 (4)	82.68 (4)
O1A^{ii}—K2—O3W	107.90 (4)	107.88 (4)	107.85 (4)	107.78 (4)	107.69 (4)
O2W—K1—N3B^{i}	149.72 (4)	149.65 (5)	149.59 (4)	149.66 (4)	149.63 (5)
O2W^{ii}—K1—N3B^{i}	120.73 (4)	120.65 (5)	120.56 (4)	120.43 (4)	120.33 (5)
O2W—K1—N3A	70.58 (4)	70.56 (5)	70.58 (4)	70.62 (4)	70.67 (4)
O2W^{ii}—K1—N3A	117.26 (4)	117.33 (4)	117.40 (4)	117.41 (4)	117.45 (4)
O2W—K1—N3A^{ii}	121.28 (4)	121.43 (4)	121.54 (4)	121.66 (4)	121.85 (4)
O2W^{ii}—K1—N3A^{ii}	65.07 (4)	64.99 (4)	64.89 (4)	64.80 (4)	64.74 (4)

O2W^{iv}—K1—N3A^{ii}	120.71 (4)	120.56 (4)	120.45 (4)	120.29 (4)	120.07 (4)
O2W—K1—N9B^{i}	138.51 (4)	138.51 (4)	138.52 (4)	138.50 (4)	138.47 (4)
O2W^{ii}—K1—N9B^{i}	83.76 (4)	83.69 (4)	83.58 (4)	83.53 (4)	83.51 (4)
O2W—K1—N9B^{iii}	83.05 (4)	82.91 (4)	82.78 (4)	82.66 (4)	82.47 (4)
O2W^{ii}—K1—N9B^{iii}	139.53 (4)	139.54 (4)	139.61 (4)	139.63 (4)	139.66 (4)
O2W^{iv}—K1—N9B^{iii}	76.68 (4)	76.72 (4)	76.79 (4)	76.84 (4)	77.00 (4)
O2W—K1—N9A	52.37 (4)	52.43 (4)	52.47 (4)	52.52 (4)	52.64 (4)
O2W^{ii}—K1—N9A	76.13 (4)	76.26 (4)	76.35 (4)	76.40 (4)	76.41 (4)
O2W^{iv}—K1—N9A	120.56 (4)	120.67 (4)	120.71 (4)	120.77 (4)	120.74 (4)
N3B^{i}—K1—O2W^{iv}	101.19 (4)	101.07 (4)	101.03 (4)	100.94 (4)	100.88 (4)
N3A—K1—O2W^{iv}	154.28 (4)	154.32 (5)	154.34 (4)	154.43 (4)	154.48 (4)
N9B^{i}—K1—O2W^{iv}	56.34 (4)	56.29 (4)	56.30 (4)	56.25 (4)	56.27 (4)

Symmetry code(s): (i) *x*+1/2, −*y*+3/2, *z*+1/2; (ii) *x*, *y*+1, *z*; (iii) *x*+1/2, −*y*+1/2, *z*+1/2; (iv) −*x*+1, −*y*, −*z*+2; (v) *x*, *y*−1, *z*; (vi) −*x*+1/2, −*y*+3/2, −*z*+1.

Table S5. Selected geometric parameters (Å). Distances between metal cations and environment for $2Na^{+}\cdot C_5H_3N_5O^{2-}\cdot 7H_2O$

	100 K	125 K	150 K	175 K	200 K	225 K	250 K	275 K	298 K
Na1—O2W	2.3413 (10)	2.3422 (9)	2.3435 (10)	2.3433 (11)	2.3459 (10)	2.3474 (11)	2.3489 (11)	2.3503 (12)	2.3505 (11)
Na1—O3W	2.4101 (10)	2.4120 (10)	2.4138 (10)	2.4158 (11)	2.4199 (11)	2.4233 (11)	2.4275 (12)	2.4347 (14)	2.4398 (13)
Na1—O4W	2.4386 (10)	2.4419 (10)	2.4434 (10)	2.4460 (11)	2.4501 (11)	2.4539 (11)	2.4574 (12)	2.4617 (13)	2.4669 (12)

Na1—O5W	2.4892 (10)	2.4904 (9)	2.4932 (10)	2.4964 (10)	2.4984 (10)	2.5008 (10)	2.5029 (11)	2.5043 (13)	2.5047 (12)
Na1—O7W^{i}	2.4380 (11)	2.4404 (10)	2.4435 (11)	2.4461 (12)	2.4515 (11)	2.4577 (11)	2.4607 (12)	2.4673 (13)	2.4732 (13)
Na1—O8W^{ii}	2.3697 (10)	2.3691 (9)	2.3713 (10)	2.3728 (10)	2.3753 (10)	2.3762 (10)	2.3793 (11)	2.3803 (12)	2.3816 (11)
Na2—O4W	2.3867 (10)	2.3871 (9)	2.3884 (10)	2.3892 (10)	2.3919 (10)	2.3928 (10)	2.3955 (11)	2.3974 (12)	2.4008 (11)
Na2—O5W	2.5035 (11)	2.5059 (10)	2.5069 (10)	2.5100 (11)	2.5104 (11)	2.5133 (11)	2.5159 (12)	2.5167 (13)	2.5178 (12)
Na2—O6W	2.3427 (10)	2.3432 (9)	2.3433 (10)	2.3460 (11)	2.3467 (11)	2.3489 (11)	2.3504 (11)	2.3532 (13)	2.3537 (12)
Na2—O6W^{iii}	2.4485 (11)	2.4516 (11)	2.4537 (11)	2.4592 (12)	2.4618 (12)	2.4661 (12)	2.4707 (13)	2.4760 (14)	2.4822 (13)
Na2—O7W	2.3581 (9)	2.3586 (9)	2.3599 (9)	2.3614 (10)	2.3625 (10)	2.3646 (10)	2.3658 (11)	2.3690 (12)	2.3701 (11)
Na2—O8W	2.4095 (9)	2.4113 (9)	2.4128 (9)	2.4148 (10)	2.4162 (10)	2.4190 (10)	2.4214 (11)	2.4245 (12)	2.4262 (11)

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 S6. Selected geometric parameters (º). Angles between metal cations and environment in $2Na^{+}\cdot C_5H_3N_5O^{2-}\cdot 7H_2O$

	100 K	125 K	150 K	175 K	200 K	225 K	250K	275 K	298 K
O2W—Na1—O3W	80.14 (3)	80.18 (3)	80.21 (4)	80.23 (4)	80.26 (4)	80.30 (4)	80.28 (4)	80.27 (5)	80.26 (4)
O2W—Na1—O4W	89.29 (3)	89.31 (3)	89.35 (3)	89.40 (4)	89.42 (4)	89.48 (4)	89.48 (4)	89.47 (5)	89.44 (4)
O2W—Na1—O5W	133.88 (4)	133.84 (3)	133.84 (4)	133.83 (4)	133.83 (4)	133.71 (4)	133.69 (4)	133.61 (5)	133.55 (4)

O2W—Na1—O7W^{i}	81.25 (4)	81.23 (3)	81.24 (4)	81.28 (4)	81.32 (4)	81.27 (4)	81.35 (4)	81.41 (5)	81.46 (4)
O2W—Na1—O8W^{ii}	129.25 (4)	129.29 (3)	129.33 (4)	129.34 (4)	129.38 (4)	129.40 (4)	129.46 (4)	129.53 (5)	129.52 (4)
O3W—Na1—O4W	82.53 (4)	82.48 (3)	82.49 (4)	82.46 (4)	82.43 (4)	82.39 (4)	82.38 (4)	82.31 (5)	82.29 (4)
O3W—Na1—O5W	136.66 (4)	136.63 (3)	136.57 (4)	136.54 (4)	136.44 (4)	136.49 (4)	136.45 (4)	136.43 (5)	136.40 (4)
O3W—Na1—O7W^{i}	137.10 (4)	137.17 (3)	137.21 (3)	137.26 (4)	137.33 (4)	137.41 (4)	137.46 (4)	137.54 (5)	137.60 (4)
O4W—Na1—O5W	73.77 (3)	73.76 (3)	73.67 (3)	73.63 (4)	73.54 (4)	73.50 (4)	73.41 (4)	73.35 (4)	73.27 (4)
O7W^{i}—Na1—O4W	135.44 (4)	135.43 (3)	135.39 (4)	135.43 (4)	135.43 (4)	135.39 (4)	135.39 (4)	135.40 (5)	135.37 (4)
O7W^{i}—Na1—O5W	81.95 (3)	81.93 (3)	81.96 (3)	81.93 (4)	81.97 (4)	81.89 (3)	81.89 (4)	81.88 (4)	81.88 (4)
O8W^{ii}—Na1—O3W	80.24 (3)	80.28 (3)	80.29 (3)	80.30 (4)	80.31 (4)	80.46 (4)	80.44 (4)	80.54 (4)	80.65 (4)
O8W^{ii}—Na1—O4W	133.33 (4)	133.30 (3)	133.26 (4)	133.19 (4)	133.14 (4)	133.17 (4)	133.08 (4)	133.05 (5)	133.14 (4)
O8W^{ii}—Na1—O5W	90.20 (3)	90.19 (3)	90.18 (3)	90.17 (4)	90.19 (4)	90.19 (4)	90.23 (4)	90.25 (4)	90.30 (4)

O8W^{ii}—Na1—O7W^{i}	82.33 (3)	82.35 (3)	82.36 (3)	82.34 (4)	82.34 (4)	82.27 (4)	82.32 (4)	82.28 (4)	82.17 (4)
O4W—Na2—O5W	74.40 (3)	74.41 (3)	74.36 (3)	74.35 (4)	74.31 (4)	74.31 (4)	74.23 (4)	74.21 (4)	74.16 (4)
O4W—Na2—O6W^{iii}	94.68 (4)	94.67 (3)	94.73 (4)	94.72 (4)	94.75 (4)	94.77 (4)	94.79 (4)	94.80 (5)	94.80 (4)
O4W—Na2—O8W	94.35 (3)	94.39 (3)	94.36 (3)	94.41 (4)	94.44 (4)	94.52 (4)	94.53 (4)	94.67 (4)	94.77 (4)
O6W—Na2—O4W	166.84 (4)	166.89 (4)	166.89 (4)	166.96 (4)	167.01 (4)	167.05 (4)	167.12 (4)	167.15 (5)	167.21 (4)
O6W—Na2—O5W	104.04 (4)	104.06 (4)	104.14 (4)	104.14 (4)	104.27 (4)	104.36 (4)	104.50 (4)	104.55 (5)	104.71 (4)
O6W^{iii}—Na2—O5W	160.28 (4)	160.30 (3)	160.31 (4)	160.33 (4)	160.37 (4)	160.41 (4)	160.38 (4)	160.46 (5)	160.47 (4)
O6W—Na2—O6W^{iii}	90.27 (4)	90.23 (3)	90.15 (4)	90.13 (4)	89.99 (4)	89.87 (4)	89.79 (4)	89.71 (5)	89.59 (4)
O6W—Na2—O7W	84.24 (3)	84.28 (3)	84.27 (3)	84.31 (4)	84.32 (4)	84.31 (4)	84.36 (4)	84.38 (5)	84.42 (4)
O6W—Na2—O8W	98.33 (3)	98.26 (3)	98.29 (3)	98.17 (4)	98.12 (4)	98.02 (4)	97.96 (4)	97.81 (4)	97.68 (4)
O7W—Na2—O4W	83.95 (3)	83.93 (3)	83.94 (3)	83.97 (4)	83.95 (4)	83.97 (4)	83.96 (4)	83.93 (4)	83.92 (4)

O7W—Na2—O5W	108.56 (3)	108.54 (3)	108.52 (3)	108.53 (4)	108.46 (4)	108.41 (4)	108.42 (4)	108.29 (4)	108.23 (4)
O7W—Na2—O6W^{iii}	86.03 (4)	86.03 (3)	86.04 (3)	85.98 (4)	85.99 (4)	86.03 (4)	86.00 (4)	86.02 (4)	86.02 (4)
O7W—Na2—O8W	169.19 (4)	169.15 (4)	169.13 (4)	169.09 (4)	169.09 (4)	169.04 (4)	169.01 (5)	169.05 (5)	168.93 (5)
O8W—Na2—O5W	81.11 (3)	81.17 (3)	81.20 (3)	81.27 (4)	81.33 (4)	81.48 (4)	81.50 (4)	81.63 (4)	81.84 (4)
O8W—Na2—O6W^{iii}	83.46 (3)	83.43 (3)	83.40 (3)	83.39 (4)	83.38 (4)	83.27 (4)	83.27 (4)	83.27 (4)	83.13 (4)
Na2—O4W—Na1	89.36 (3)	89.36 (3)	89.42 (3)	89.47 (4)	89.48 (4)	89.48 (4)	89.51 (4)	89.53 (4)	89.47 (4)
Na1—O5W—Na2	85.62 (3)	85.63 (3)	85.67 (3)	85.66 (3)	85.77 (3)	85.75 (3)	85.82 (4)	85.93 (4)	86.03 (4)
Na2—O6W—Na2^{iii}	89.73 (4)	89.78 (3)	89.85 (4)	89.86 (4)	90.01 (4)	90.13 (4)	90.21 (4)	90.29 (5)	90.41 (4)
Na2—O7W—Na1^{iv}	119.02 (4)	118.99 (4)	118.96 (4)	118.95 (4)	118.89 (4)	118.79 (4)	118.80 (5)	118.65 (5)	118.64 (5)
Na1^{v}—O8W—Na2	105.41 (4)	105.45 (3)	105.41 (4)	105.45 (4)	105.47 (4)	105.52 (4)	105.53 (4)	105.60 (4)	105.73 (4)

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

3. Anisotropy of lattice strain on temperature variations

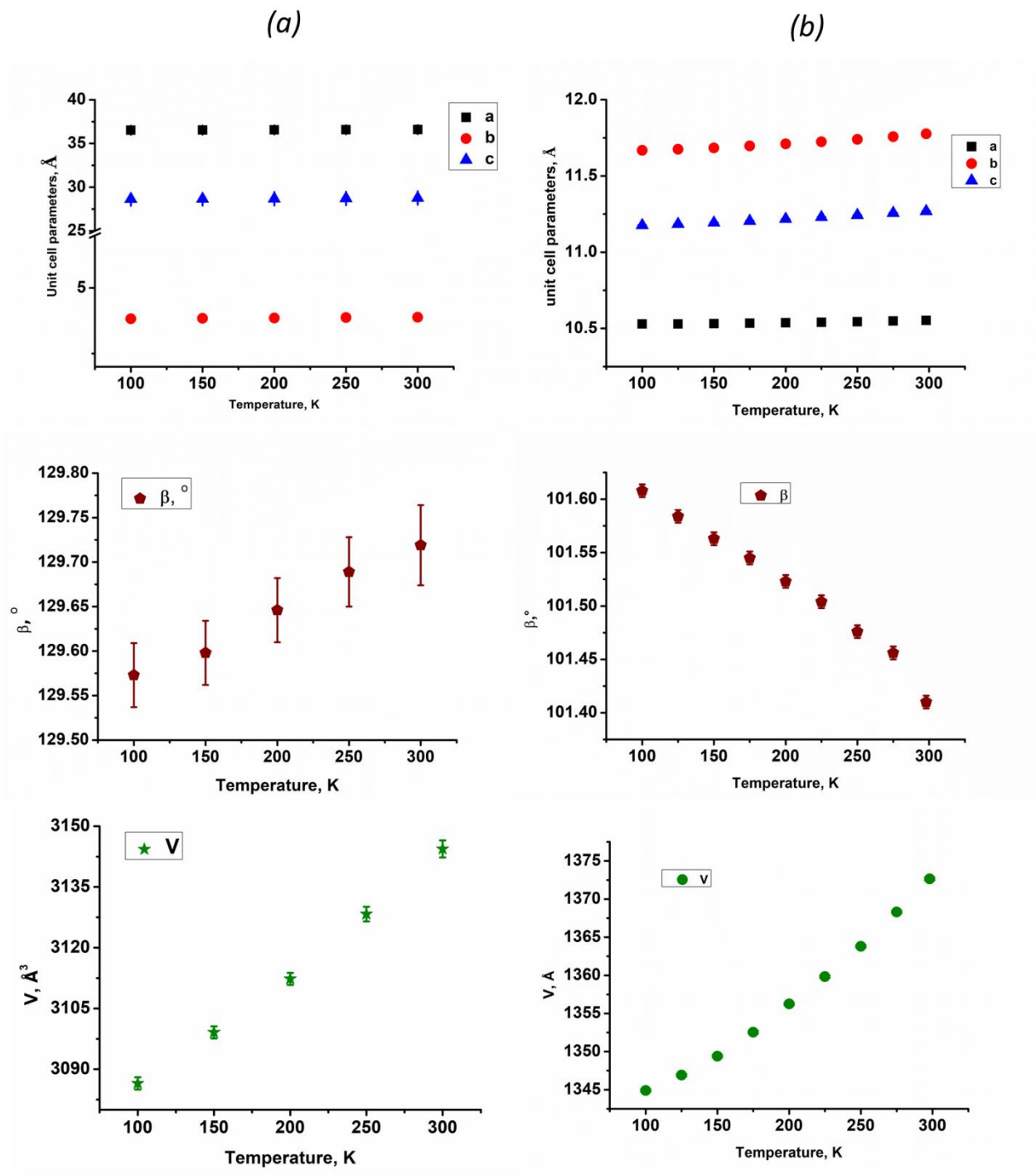

Figure S2. The changes in the unit cell parameters and volume *vs* temperature for the two salts: $K^{+}\cdot C_5H_4N_5O^{-}\cdot H_2O$ (a) and $2Na^{+}\cdot C_5H_3N_5O^{2-}\cdot 7H_2O$ (b).

ThetaToTensor software was used to calculate thermal expansion tensors and to represent graphically its characteristic surface (Bubnova et al., 2013).

The values of thermal expansion coefficients along the crystallographic axes *a*, *b*, *c* (α_a, α_b, α_c) and the temperature dependence of the β angle (α_β) for both salts were compared (Tables S7 & S8).

The deformation of the (*a x c*) plane was controlled mostly by the change in β. The α_β values for these two salts are opposite in sign to each other and differ by magnitude twice ($5.93 \cdot 10^{-6}$ K^{-1} for potassium salt; $-9.19 \cdot 10^{-6}$ K^{-1} for sodium salt), so that the β angle for potassium salt decreases quite strongly as the temperature increases. The values of the thermal expansion coefficients along the crystallographic axes *a, b, c* ($\alpha_a, \alpha_b, \alpha_c$) also differ dramatically for these two salts. For potassium salt one can conclude that the structure is the most compressible along b axis, α_b ~ 3 times higher than α_c ($73.1 \cdot 10^{-6}$ K^{-1} and $20.9 \cdot 10^{-6}$ K^{-1} respectively). This makes sense: the direction along *b* axis corresponds to the axis of the channels, while the chains in the c direction formed by coordination polyhedra of either guanine, or K-O clusters, should be more rigid. The structure is the least compressible in the third crystallographic direction - α_a is approximately 7 times smaller than α_b. This direction corresponds to the layers of the guanine fragments and K-O polyhedra of different types, and the structure could be predicted to be rigid in this direction. For the sodium salt one can conclude that the directions along b and c axes are close to each other by compressibility, while the coefficient α_a is four times smaller. The structure is the least compressible in the direction normal to the axes of the channels. The similarity of thermal expansion in the directions b and c can be understood better, if we remove the guanine molecules from the figure - Figure 3d, to make the Na-O polyhedra ring-like motifs more clearly visible.

The shift components of the tensor for each salt practically do not change with temperature (for sodium salt: α_{11} $-6.6 \cdot 10^{-6}$ K^{-1}, α_{33} $10.0 \cdot 10^{-6}$ K^{-1}, μ_{c3} 50.8°; for potassium salt α_{11} $3.2 \cdot 10^{-6}$ K^{-1}, α_{33} $-14.2 \cdot 10^{-6}$ K^{-1}, μ_{c3} 64.8°).

Table S7. Values of the expansion tensor coefficient for the potassium salt of guanine, multiplied by 10^6 (K^{-1})

T, K	100	150	200	250	300
α_{11}	-1.482(53)	-1.503(53)	-1.523(54)	-1.543(55)	-1.563(56)
α_{22}	73.1(2.6)	72.8(2.6)	72.6(2.5)	72.3(2.5)	72.0(2.5)
α_{33}	21.09(76)	21.07(75)	21.04(75)	21.02(75)	21.00(75)
μ_{a1}, °	45.0	45.0	45.1	45.1	45.2
μ_{c3},°	5.4	5.4	5.4	5.4	5.4

α_a	9.80(51)	9.80(51)	9.79(51)	9.79(51)	9.78(51)
α_b	73.1(1.4)	72.8(1.4)	72.6(1.4)	72.3(1.4)	72.0(1.4)
α_c	20.9(1.7)	20.9(1.6)	20.8(1.6)	20.8(1.6)	20.8(1.6)
α_β	5.93(35)	5.93(35)	5.93(35)	5.93(35)	5.92(35)
α_V	92.7(3.3)	92.4(3.3)	92.1(3.2)	91.8(3.2)	91.5(3.2)

The orientation of the axes of the expansion tensor for monoclinic crystals is defined as follows: α_{22} axis is along the *b* axis, two other axes are determined by the angles $\mu_{a1,}$ $\mu_{c3.}$ (for example, μ_{c3} = angle between *c* axis and α_{33}). The coefficients $\alpha_{a,}$ $\alpha_{b,}$ α_c correspond to the values of thermal expansion coefficients along the crystallographic axis *a, b, c*; α_β - corresponds to the value of thermal expansion coefficients of angle β; α_V - corresponds to the value of bulk thermal expansion coefficient. All α coefficients are given in K^{-1}.

Table S8 Values of the expansion tensor coefficient for the sodium salt of guanine, multiplied by 10^6 (K^{-1})

T, K	100	125	150	175	200	225	250	275	298
α_{11}	11.01(49)	11.00(49)	11.00(49)	10.99(49)	10.98(49)	10.97(49)	10.97(49)	10.96(49)	10.95(49)
α_{22}	47.1(2.1)	47.1(2.1)	47.0(2)	47.0(2)	46.9(2)	46.8(2)	46.8(2)	46.7(2)	46.7(2)
α_{33}	46.7(2)	46.7(2)	46.6(2)	46.6(2)	46.5(2)	46.5(2)	46.4(2)	46.4(2)	46.4(2)
$\mu_{a1,}$ °	8.1	8.1	8.1	8.2	8.2	8.2	8.2	8.3	8.3
$\mu_{c3,}$ °	19.7	19.7	19.7	19.7	19.7	19.7	19.7	19.7	19.7
α_a	11.72(	11.71(8	11.71(8	11.71(8	11.70(8	11.70(8	11.70(8	11.69(8	11.69(8

	85)	5)	5)	5)	5)	5)	5)	5)	5)
α_b	47.1(2.3)	47.1(2.3)	47.0(2.3)	47.0(2.3)	46.9(2.3)	46.8(2.3)	46.8(2.3)	46.7(2.3)	46.7(2.3)
α_c	42.7(1.3)	42.6(1.3)	42.6(1.3)	42.5(1.3)	42.5(1.3)	42.5(1.3)	42.4(1.3)	42.4(1.3)	42.3(1.3)
α_β	-9.19(43)	-9.19(43)	-9.20(43)	-9.20(43)	-9.20(43)	-9.20(43)	-9.21(43)	-9.21(43)	-9.21(43)
α_V	104.9(4.6)	104.8(4.6)	104.6(4.6)	104.5(4.6)	104.4(4.5)	104.3(4.5)	104.2(4.5)	104.1(4.5)	104.0(4.5)

The temperature dependence of the distances between the planes, in which the neighbouring guanine anions are located, is plotted in Figure S3. There are two different types of planes in the potassium salt of guanine, depending on the type of guanine anion (G1 or G7). The distance between G1-planes is slightly longer than that between the G7-planes (~ 3.555 Å and 3.408 Å at 300 K, respectively). For a comparison, the interplanar distances in the structure of sodium salt of guanine heptahydrate are equal to 3.474 Å and 2.014 Å (Gaydamaka et al., 2019). In the structure of the guanine monohydrate (Thewalt et al., 1971) all the guanine molecules are stacked along the c axis with an interplanar spacing of 3.30 Å. The base-pair spacing in the DNA of A and B types is equal to 2.925 Å and 3.35 Å, respectively (Kahn et al., 2007). In the temperature range of 100 K - 300 K G1 and G7 distances increase approximately at 1 %, while distances between the planes in the sodium salt change in the opposite direction: one increases (~ 1,6 %), another one decreases (~ -1.7%) - the same trend was observed for the structural changes in the sodium salt on hydrostatic compression.

For the potassium salt, the largest relative changes in the distances of the hydrogen bonds were observed for the bonds along b axis: the two bonds connecting guanine anions directly – N2a…N3b (relative change ~1.2%), N1b…O1 (1%), and the bond connecting guanine with water (O3w…N7b^{iii} (1 %). The relative changes in the distances of the hydrogen bonds for sodium salt were more significant: the largest relative change was observed for the bond connecting guanine with water O4w…N9 (7.1 %), one of the bond connecting two water molecules: O3w..O5w'' (1.88 %), O6w…O2w' (1%) and one the bond connecting carbonyl group of guanine with water

O5w…O1^{v} (1.09 %). It is interesting to note that the bonds O4w…N9 and O5w…O1v connect guanine anion with water from the opposite sites.

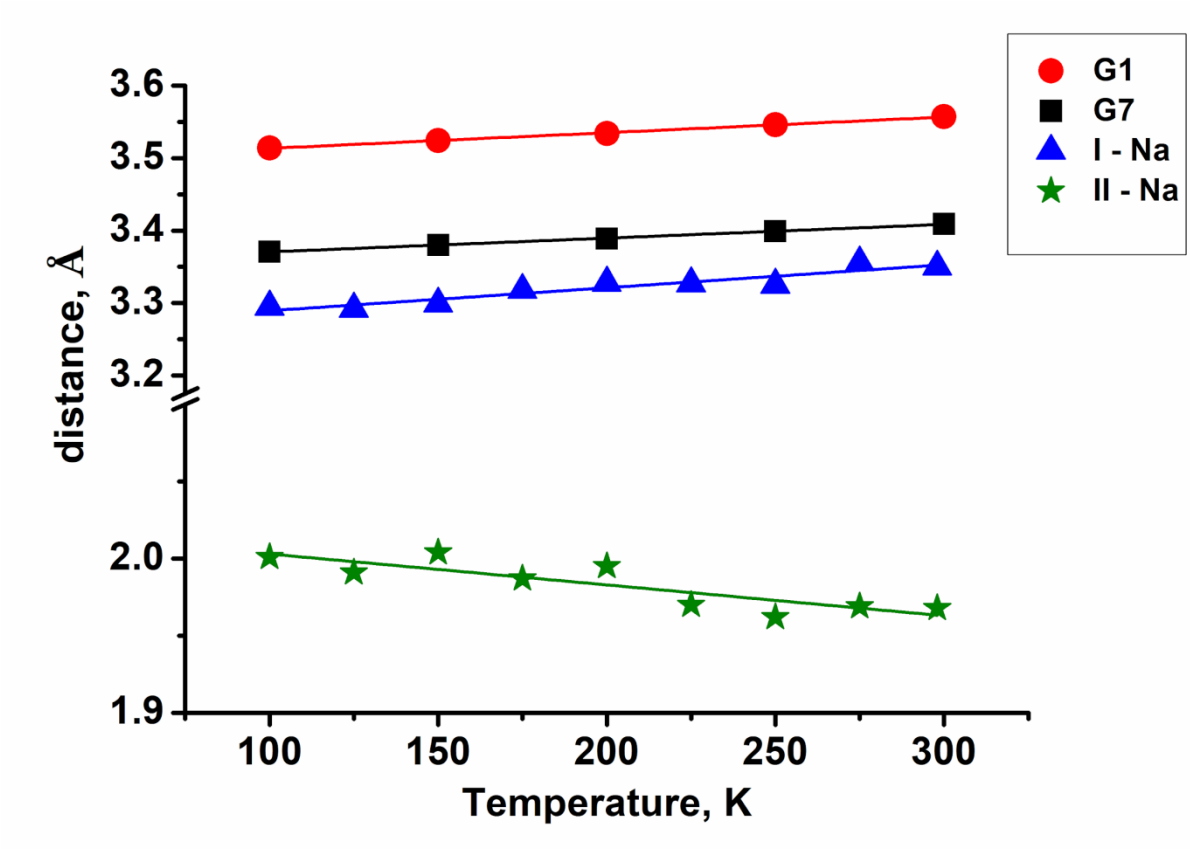

Figure S3. Distances between alternating planes corresponding to the neighbouring guanine anions in both salts

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