Supporting Information

Solvothermal Synthesis, Crystal Growth, and Structure Determination of Sodium and Potassium Guanidinate

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S1: DFT-optimized fractional coordinates of all H atoms in $NaCN_3H_4$ and their corresponding N–H bond lengths (Å).

	x	*y*	*z*	*d*(N–H)	bonded to
H1	0.8300	0.6490	0.9124	1.036	N1
H2	0.9515	0.4211	0.8535	1.025	N1
H3	0.9497	0.4491	0.6225	1.024	N2
H4	0.6061	0.8819	0.5487	1.025	N3

S2: DFT-optimized fractional coordinates of all H atoms in KCN_3H_4 and their corresponding N–H bond lengths (Å).

	x	*y*	*z*	*d*(N–H)	bonded to
H1	0.2245	0.7660	0.4866	1.021	N1
H2	0.4115	0.6315	0.5062	1.035	N1
H3	0.4836	0.4428	0.4032	1.030	N2
H4	0.2556	0.6377	0.3777	1.028	N3
H5	0.5622	0.2638	0.3278	1.019	N4
H6	0.7520	0.1994	0.3645	1.033	N4
H7	0.6121	0.7168	0.3639	1.027	N5
H8	0.3919	0.8023	0.3136	1.031	N6
H9	0.2865	0.6189	0.2269	1.021	N7
H10	0.0853	0.7383	0.2343	1.023	N7
H11	0.0132	0.4779	0.3306	1.028	N8
H12	0.3062	0.3812	0.3252	1.025	N9
H13	0.8772	0.9662	0.4744	1.030	N10
H14	0.8091	0.9815	0.4183	1.041	N10
H15	0.1168	0.3479	0.3990	1.026	N11
H16	0.2004	0.3410	0.4703	1.027	N12

S3: Experimental (XRD) and theoretical (DFT) amino H–N–H angles in the guanidinate anions of $NaCN_3H_4$ and KCN_3H_4.

		XRD (°)	DFT (°)
$NaCN_3H_4$	H1–N1–H2	114(1)	112.6
KCN_3H_4	H1–N1–H2	111(2)	113.9
	H5–N4–H6	116(2)	113.9
	H9–N7–H10	111(2)	113.1
	H13–N10–H14	114(2)	111.4