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Supporting information for article:

Low-temperature phase transition and high-pressure phase stability of 1*H*-pyrazole-1carboxamidine nitrate

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Supporting information

Table S1 Experimental frequencies (cm^{-1}) taken from Raman and IR spectra collected at various temperature conditions and assignment of the bands.

$\nu_{exp,\ R}$ 300K	$\nu_{exp,\ IR}$ 300K	$\nu_{exp,\ IR}$ 112K	$\nu_{exp,\ IR}$ 12K	Assignment
	3322	3318	3315	νNH
3145	3143	3146	3149	νCH
3125		3127	3129	νCH
3105				νCH
3065				$\nu_{as}NH_2$
	1707	1712	1713	$\nu_{as}CN_{(gua)}$
1656	1658	1662	1665	$\nu_{as}CN_{(gua)}$
1563	1573	1581	1584	$\delta_s NH_2$
1537		1562	1561	$\delta_s NH_2$
			1419	$\nu_3 NO_3$
1409	1409	1409	1407	$\nu_3 NO_3$
1389	1386	1388	1387	$\nu_3 NO_3$
			1316	νCN
1309	1309	1310	1310	νCN
		1299	1298	νCN
1228	1231	1234	1232	νCN + νCC
1212	1216	1217	1217	νNN + δCH

			1122	ρNH_2
1109	1099	1102	1102	$\delta CH + \rho NH_2$
1087				$\delta CH + \rho NH_2$
1065				$\nu_1 NO_3$
	1064	1071	1074	δCH
1044	1041	1041	1040	δCH
946	940	943	945	$\delta CH + \delta CNN$
	919			ring breathing
908	910	912	912	ring breathing
881	886	888	888	γCH
	824	823	824	$\nu_2 NO_3$
		789	792	$\nu_4 NO_3$
	780	780	780	$\nu_4 NO_3$
722	722	721	723	$\tau NH_2 + \gamma NH_2$
		706	708	$\gamma CN_{(gua)}$
687	668	655	657	$\gamma CN_{(gua)}$
634		597	600	γCCN
584		551	558	γCCN

Table S2 Hydrogen-bond geometry (Å, º) for $(HPyCA)NO_3$ at 300 and 100 K.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
300 K				
N3—H3A···O1^{i}	0.86	1.92	2.7726 (17)	174.4
N3—H3B···N2^{ii}	0.86	2.25	2.9887 (17)	144.5
N4—H4A···O3^{i}	0.86	2.10	2.9506 (19)	170.6
N4—H4B···O3^{iii}	0.86	2.42	3.2752 (18)	170.4
100 K				
N13—H13A···O12	0.86	1.91	2.7628 (14)	172.3
N13—H13B···N12^{iv}	0.86	2.23	2.9607 (17)	143.4
N14—H14A···O11	0.86	2.06	2.9188 (15)	172.3
N14—H14B···O22	0.86	2.71	3.5663 (15)	177.4
N14—H14B···O23	0.86	2.19	2.7864 (16)	126.4
N23—H23A···O21	0.86	1.93	2.7834 (13)	174.4

N23—H23B···N22^{v}	0.86	2.21	2.9493 (18)	143.8
N24—H24A···O22	0.86	2.07	2.9191 (13)	168.1
N24—H24B···O11^{vi}	0.86	2.19	3.0253 (15)	163.6

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

Table S3 Hydrogen-bond geometry (Å, º) for (HPyCA)NO_3 at 0.67 GPa and 0.89 GPa.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
0.67 GPa				
N3—H3A···O1^{iii}	0.86	1.91	2.757 (5)	169.7
N3—H3B···N2^{iv}	0.86	2.22	2.956 (7)	142.8
N4—H4A···O3^{iii}	0.86	2.11	2.966 (6)	173.2
N4—H4B···O3^{ii}	0.86	2.37	3.214 (6)	169.2
0.89 GPa				
N3—H3A···O1^{iii}	0.86	1.92	2.769 (6)	168.4
N3—H3B···N2^{iv}	0.86	2.22	2.942 (8)	142.0
N4—H4A···O3^{iii}	0.86	2.11	2.968 (6)	173.2
N4—H4B···O3^{ii}	0.86	2.36	3.209 (7)	169.0

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

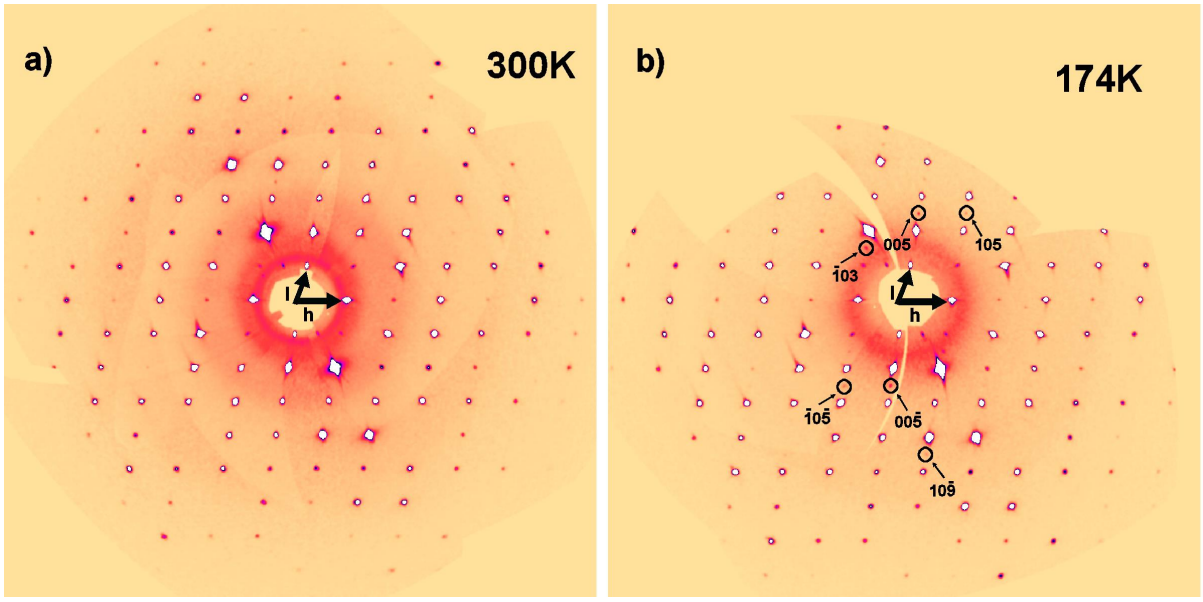

Figure S1 A comparison of diffraction pattern on the (h0l) plane obtained (a) at 300 K and (b) at 174 K. Additional l odd reflections indicate a disappearance of the *c* glide plane.

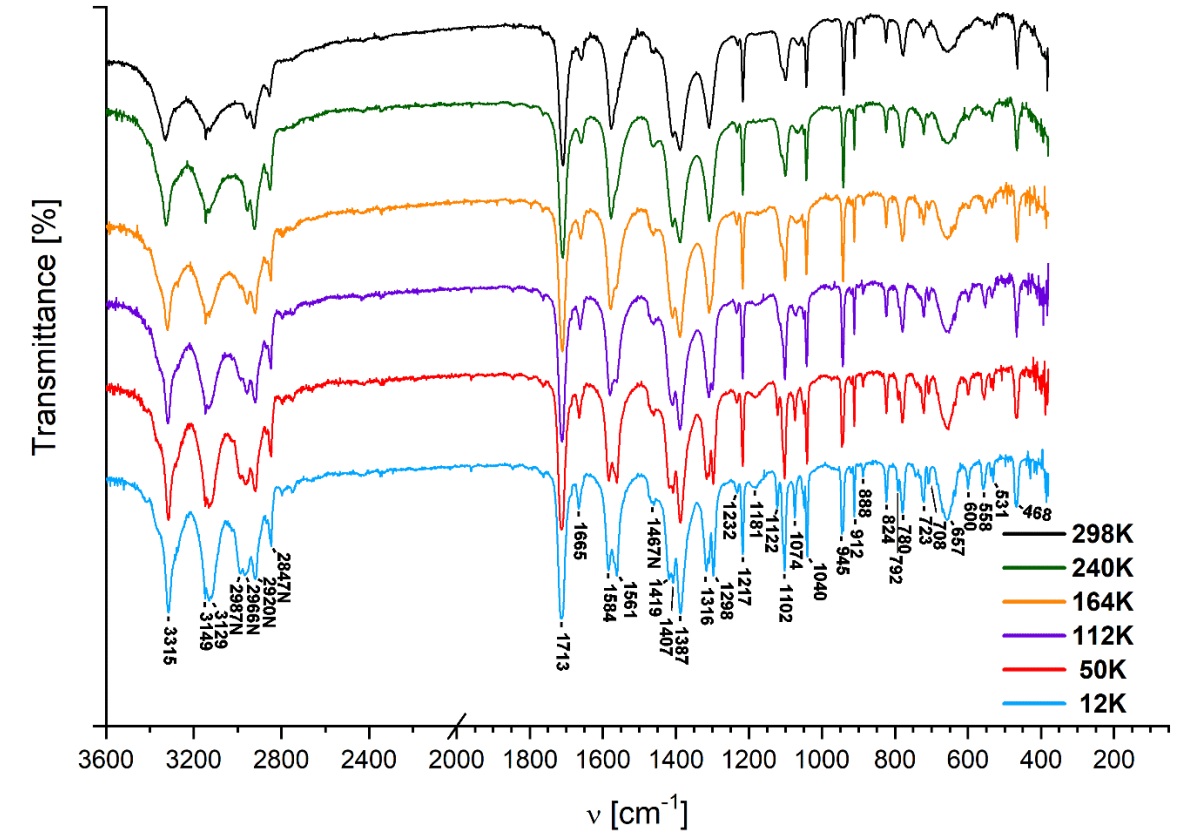

Figure S2 IR spectra collected for (HPyCA)NO_3 in the range of 300-12 K upon cooling the sample.

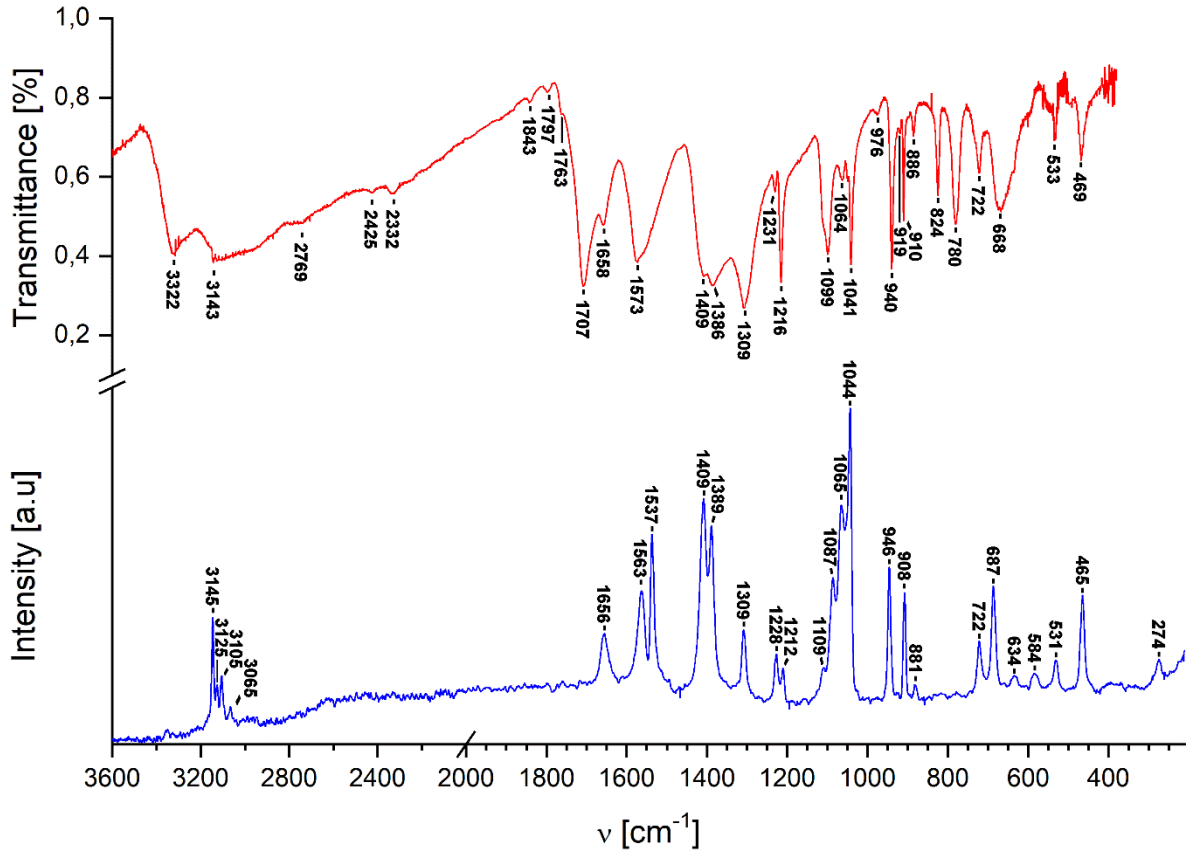

Figure S3 IR and Raman spectra collected for (HPyCA)NO_3 at ambient conditions.

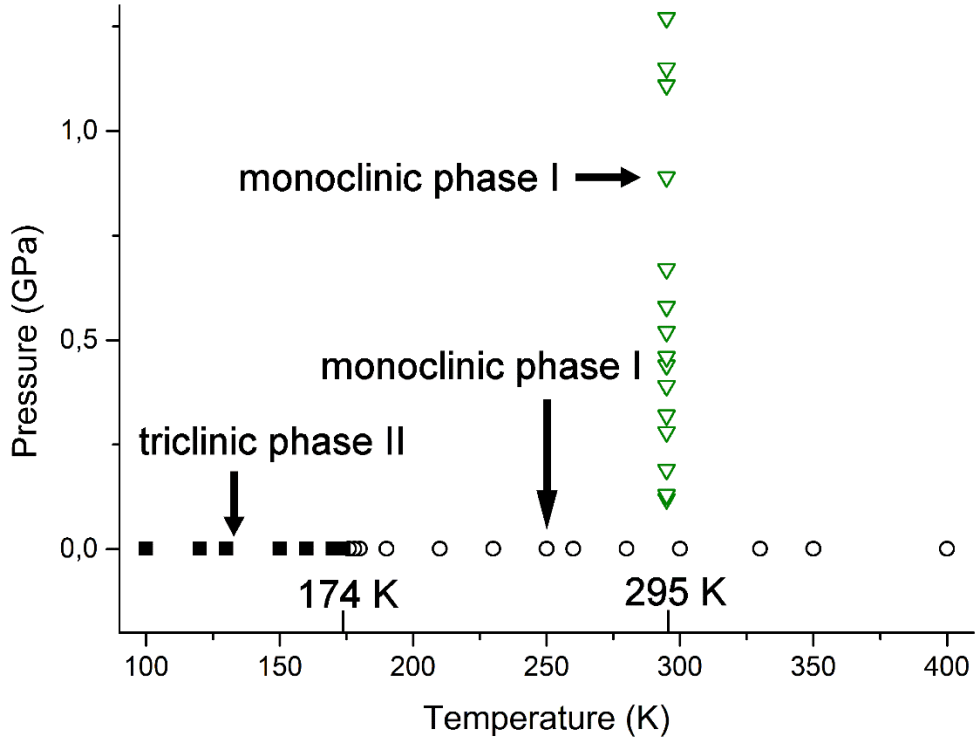

Figure S4 Phase diagram for (HPyCA)NO_3