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Elastic properties and acoustic dissipation associated with a disorder-order ferroelectric transition in a metal-organic framework

Zhiying Zhang[a,b,*], Wei Li[c,*], Michael A. Carpenter[b], Christopher J. Howard[d], Anthony K. Cheetham[c]

[a]*Department of Metallic Materials, School of Materials Science and Engineering, Wuhan University of Technology, 122 Luoshi Road, Wuhan, Hubei, 430070, China*

[b]*Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge, CB2 3EQ, United Kingdom*

[c]*Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge, CB3 0FS, United Kingdom*

[d]*School of Engineering, University of Newcastle, New South Wales, 2308, Australia*

***To whom correspondence should be addressed. E-mail: zhiyingzhang@whut.edu.cn, wl276@cam.ac.uk**

Table S1. Crystallographic data of frmaework **1** determined at 300 and 120 K.

Moiety formula	$[NH_4][Zn(HCOO)_3]$	
Formula weight	208.18	
Temperature / K	300	120
Crystal system	Hexagonal	Hexagonal
Phase	Paraelectric	Ferroelectric
Space group	$P6_322$	$P6_3$
a / Å	7.3090(2)	12.5946(3)
b / Å	7.3090(2)	12.5946(3)
c / Å	8.1701(3)	8.2087(3)
α / º	90.00	90.00
β / º	90.00	90.00
γ / º	120.00	120.00
V / Å^3	377.98(2)	1127.65(6)
Z	2	6
ρ_c / g cm^{-3}	1.920	1.930
μ / mm^{-1}	3.235	3.253
Flack parameter	-0.04(3)	0.07(2)
GOF on F^2	1.074	1.087
R_1, $[I > 2\sigma(I)]^a$	0.0180	0.0276
wR_2, $[I > 2\sigma(I)]^b$	0.0487	0.0845
$^aR_1 = \Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$ $^bwR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$		

Table S2. Hydrogen bond distances (Å) and bond angles (°) of **1** at 300 and 120 K.

Tem/K	N–H•••O	$d_{N–H}$ / Å	$d_{H\cdots O}$ / Å	$d_{N\cdots O}$ / Å	< NHO
300	N1–H1A•••O1	1.08(2)	1.934(2)	2.971(3)	160(1)
120	N1–H1B•••O2^{i}	0.99(1)	1.885(2)	2.866(3)	176(2)
	N2–H2B•••O4^{ii}	0.99(1)	1.844(2)	2.829(3)	176(2)
	N3–H3A•••O5^{iii}	0.98(1)	1.900(2)	2.857(3)	166(2)

Symmetry codes: i, y-1, -x+y, z-0.5; ii, -x+y, 1-x, z-1; iii, 2+x-y, 1+x, z-0.5.

Table S3. Variable-pressure lattice parameter data of frameworks **1** and **2**, determined using synchrotron single-crystal X-ray diffraction**.**

Phase	Tem / K	*a* / Å	*b* / Å	*c* / Å	*V* / Å^3
Paraelectric $P6_322$	120	12.5946(3)	12.5946(3)	8.2087(3)	1127.65(6)
	130	12.5978(4)	12.5978(4)	8.2008(3)	1127.13(6)
	140	12.6002(4)	12.6002(4)	8.1991(3)	1127.33(6)
	150	12.6053(4)	12.6053(4)	8.1987(3)	1128.19(6)
	160	12.6069(4)	12.6069(4)	8.1951(3)	1127.99(6)
	170	12.6130(4)	12.6130(4)	8.1939(3)	1128.91(6)
	180	12.6169(4)	12.6169(4)	8.1906(3)	1129.15(6)
Ferroelectric $P6_3$	190	7.2911(2)	7.2911(2)	8.1904	377.03(6)
	200	7.2940(3)	7.2940(3)	8.1873	377.22(7)
	210	7.2956(3)	7.2956(3)	8.184	377.24(7)
	220	7.2975(3)	7.2975(3)	8.1834	377.41(6)
	230	7.2992(3)	7.2992(3)	8.1813	377.49(6)
	240	7.3008(3)	7.3008(3)	8.179	377.55(6)
	250	7.3024(3)	7.3024(3)	8.1773	377.64(6)
	260	7.3034(3)	7.3034(3)	8.1757	377.66(6)
	270	7.3047(3)	7.3047(3)	8.1746	377.74(6)
	280	7.3057(3)	7.3057(3)	8.1729	377.78(6)
	290	7.3078(3)	7.3078(3)	8.1715	377.92(6)
	300	7.3090(2)	7.3090(2)	8.1701(3)	377.98(2)