Supporting Information for

Negative thermal expansion and linear compressibility in 1H-imidazol-3-ium 2-hydroxybenzoate with a helical network of hydrogen bonds

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Figure S1. The second (red) and third-order (blue) Birch-Murnaghan equation of state for **SalImi**.

Figure S2. Two projections of chains of molecules linked by hydrogen bonds C3a–H3aa···O10b^{ii} into layers parallel to the *ab* plane.

Figure S3. A view of the unit cell of **SalImi** showing the double layers of molecules parallel to the *ab* plane. Adjacent double layers are shown in black and gray for clarity of drawing. The symmetry codes are explained in Table 1 and Fig. 3. *Cg*1 is a phenylene ring centroid; Ph and Im are phenylenes and imidazolium rings. Symmetry codes: (iii) 3/2–*x*,1–*y*,1/2+*z*, (iv) 1–x,1–y,1–z.

Figure S4. (a) The C–H···*Cg* and (b) π···π interactions; the shaded area highlights the degree of overlap of the Ph and Im rings; *Cg*1 is phenylene ring centroid; Ph and Im are phenylene and imidazolium rings. H atoms not involved in hydrogen bonding have been omitted for clarity. Symmetry code: (iv) 1–x, 1–y, 1–z.

Figure S5. Raman spectra of imidazolium salicylate under temperature in three spectral regions: 20–220 (left), 760–920 (middle), and 1420–1660 cm^{-1} (right).

Figure S6. Raman spectra of imidazolium salicylate under pressure in two spectral regions: 950–650 (left) and 180–50 cm^{-1} (right).

Figure S7. Calculated FT-IR (a) and Raman (b) spectra of imidazolium and acid ions; scaling factor of 0.97, DFT method: ωB97XD/6-311++G(d,p).

Figure S8. Temperature evolution of the lengths of C···O in the C−H···O hydrogen bond (a) and O···O in the O−H···O hydrogen bond (b). The evolution of the position of the bands at 757 and 768cm^{-1} (a) and 1346cm^{-1} (b) is shown on the right.

Figure S9. Pressure evolution of C···O lengths in C−H···O hydrogen bond (a) and O···O in O−H···O hydrogen bond (b).

Figure S10. Crystal structure of imidazolium salicylate. The dotted lines denote the axes where the imidazolium ion rotates in the crystal.

Figure S11. Values of anharmonic factor ψ(A) (a), damping parameter $\Delta\nu/\nu_0$, and the maximum absorption energy $F[A_c(\nu_0)]$ (b) of imidazolium salicylate as a function of temperature.

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Table S1. Crystal data, data collection, and structure refinement for **SalImi** at different temperatures at atmospheric pressure.

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Table S4. Cell parameters (Å, °) for **SalImi** at different pressures (GPa).

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Table S6. Hydrogen-bonds and C—H···*Cg* interactions (Å, °) in the crystal structure of **SalImi** at different temperatures.

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Table S8. SalImi QTAiM parameters (in atomic unit) as a function of temperature corresponding to the H···O bond critical point (BCPs), the electron density at BCP ρ_{BCP}; Laplacian of electron density at BCP, $\Delta\rho_{BCP}$; total electron energy density at BCP, H_{BCP} and the components of the H_{BCP}: kinetic electron energy density, G_{BCP}; potential electron energy density, V_{BCP}, the hydrogen bond energy, E_{HB} (kcal·mol^{-1}).

Table S9. SalImi QTAiM parameters (in atomic unit) as a function of pressure corresponding to the H···O bond critical point (BCPs), the electron density at BCP ρ_{BCP}; Laplacian of electron density at BCP, $\Delta^2\rho_{BCP}$; total electron energy density at BCP, H_{BCP} and the components of the H_{BCP}: kinetic electron energy density, G_{BCP}; potential electron energy density, V_{BCP}, the hydrogen bond energy, E_{HB}.

Table S10. Parameters of the helicoid: a_h (semi-major axis), b_h (semi-minor axis), Sh_h (helix pitch), c_h (focal length of the ellipse), e_h (eccentricity of the ellipse), l_h (circumference of the ellipse), and S_h (area of the ellipse).

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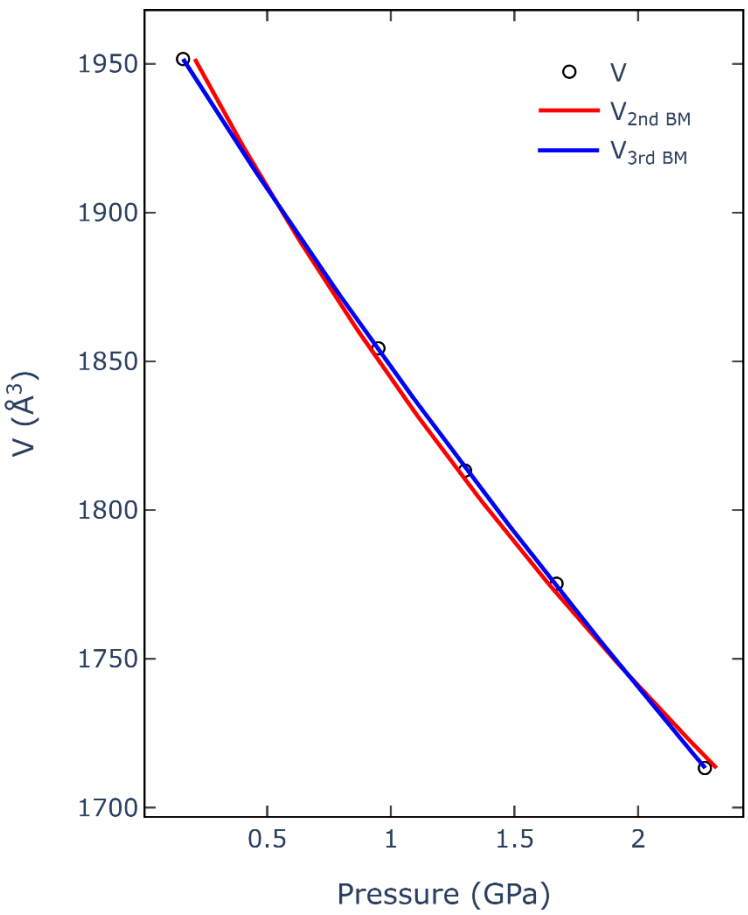
Table S14. Lengths and angles of the bonds in the imidazole ion as a function of the pressure. Note: The atomic labeling scheme is shown in Figure 1.



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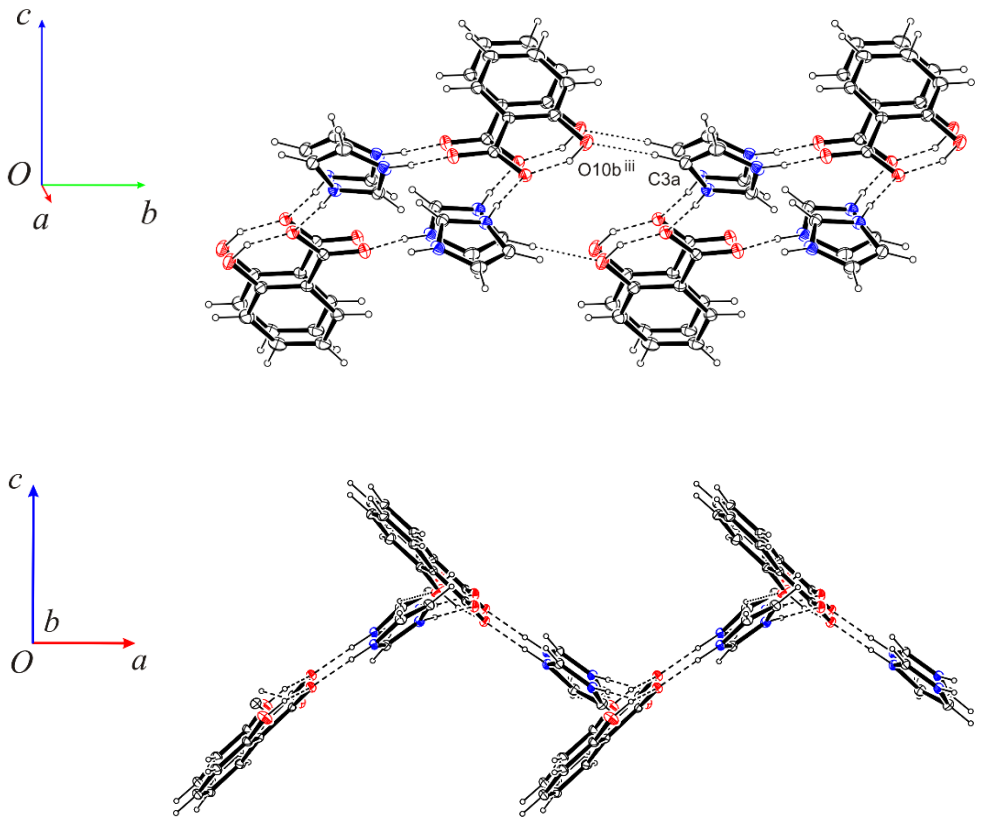

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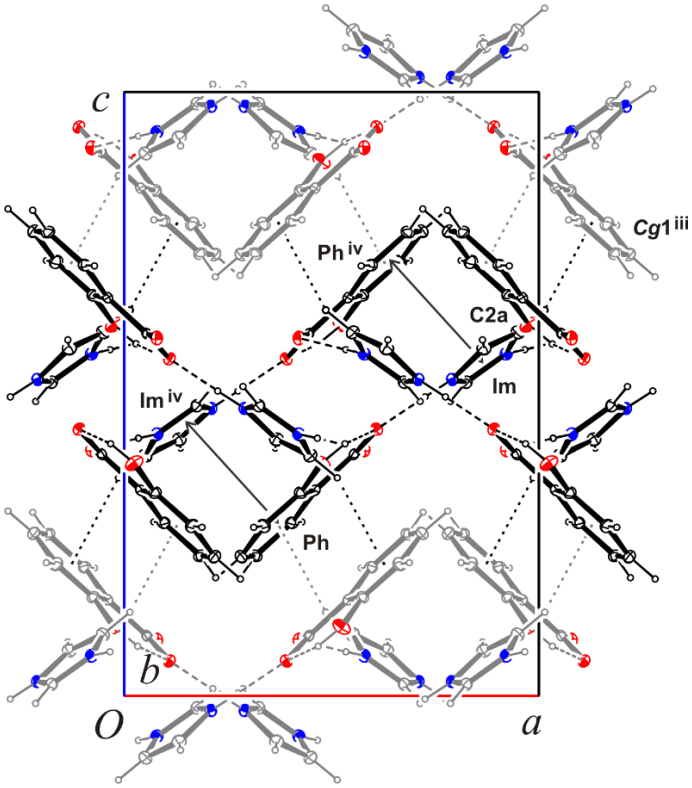

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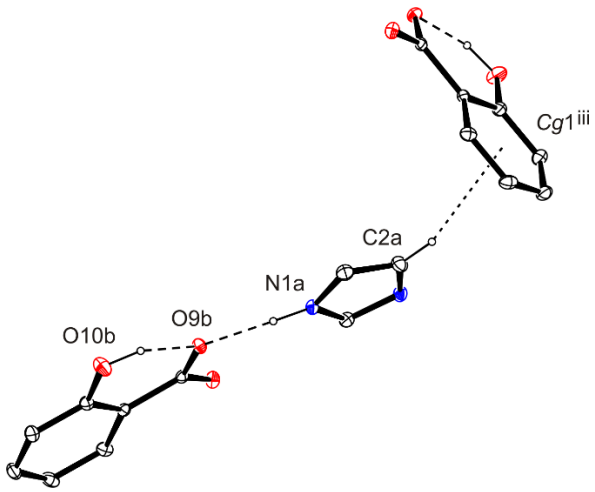
a)



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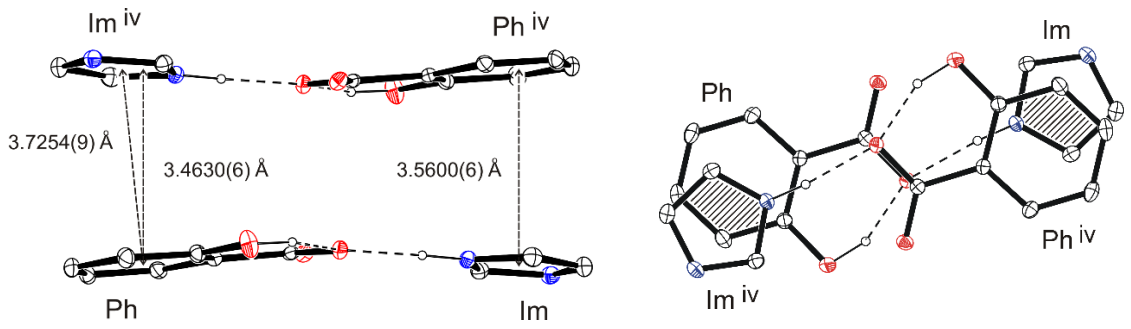

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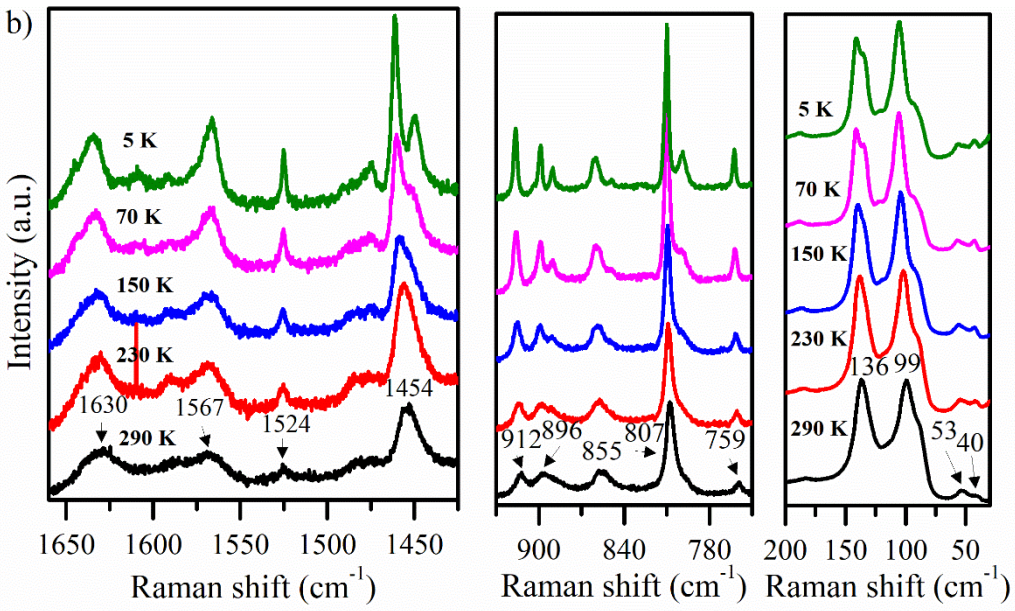

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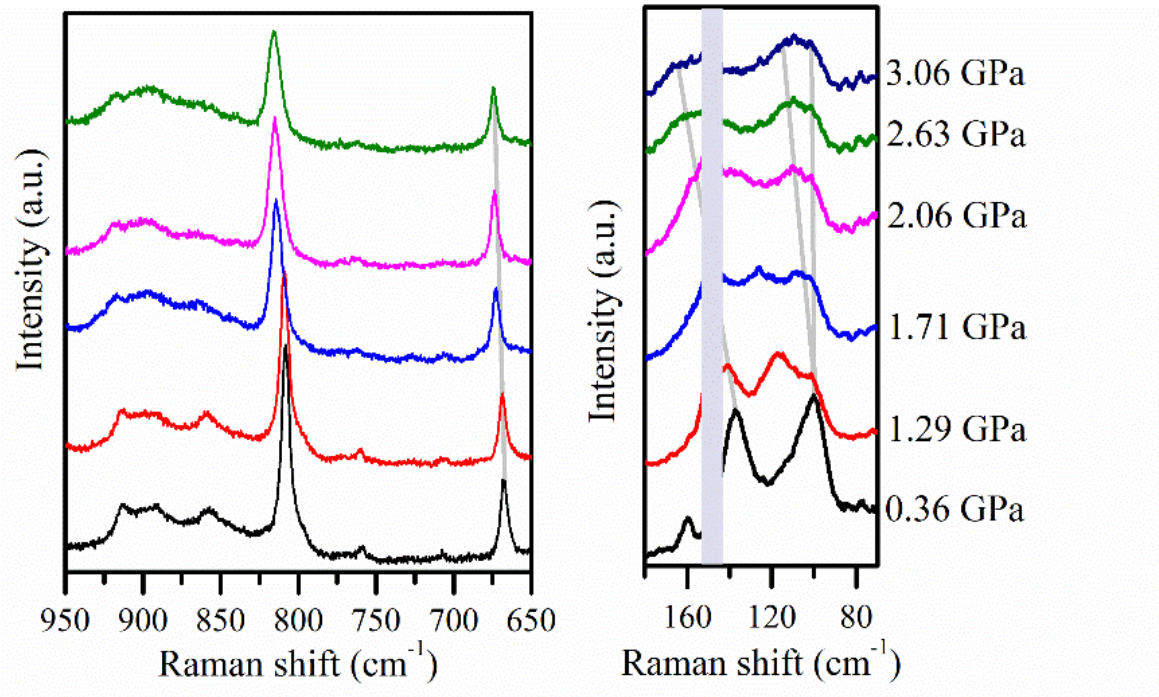

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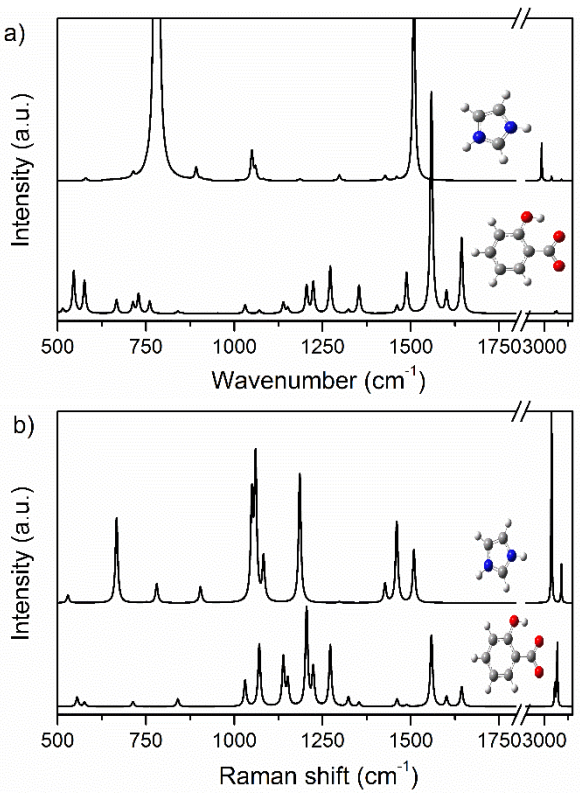

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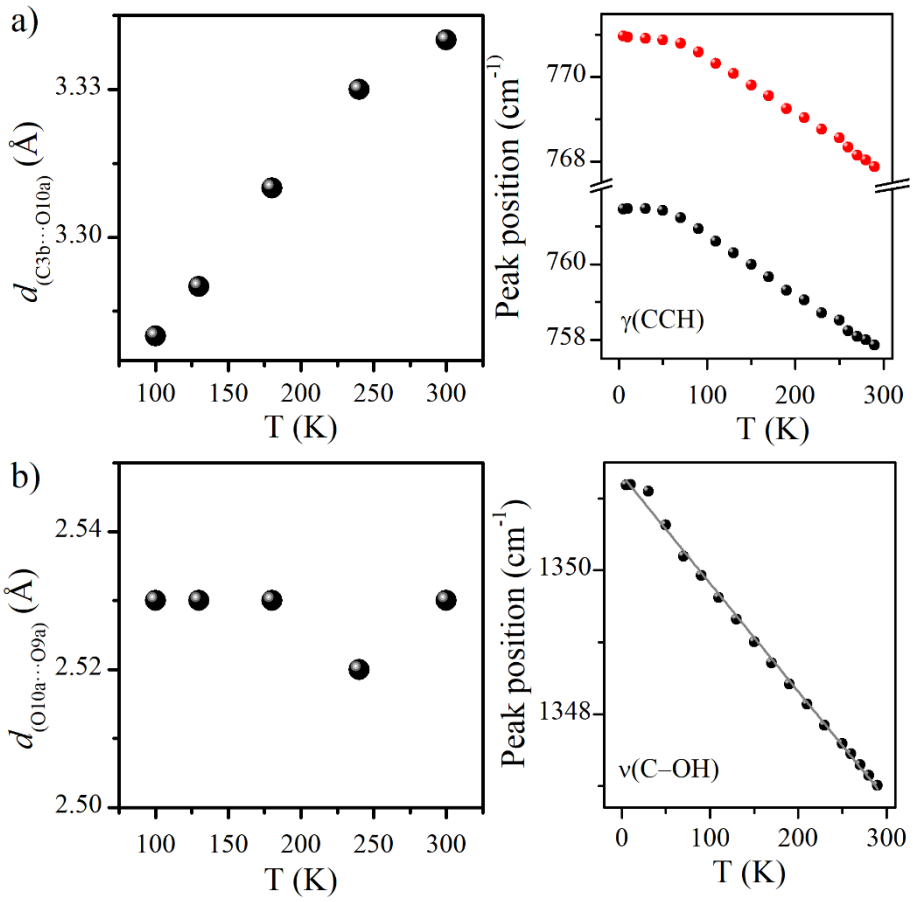

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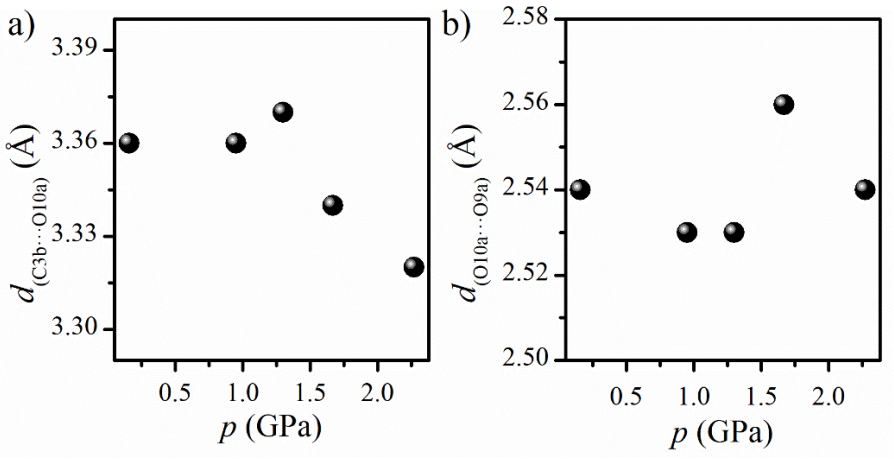

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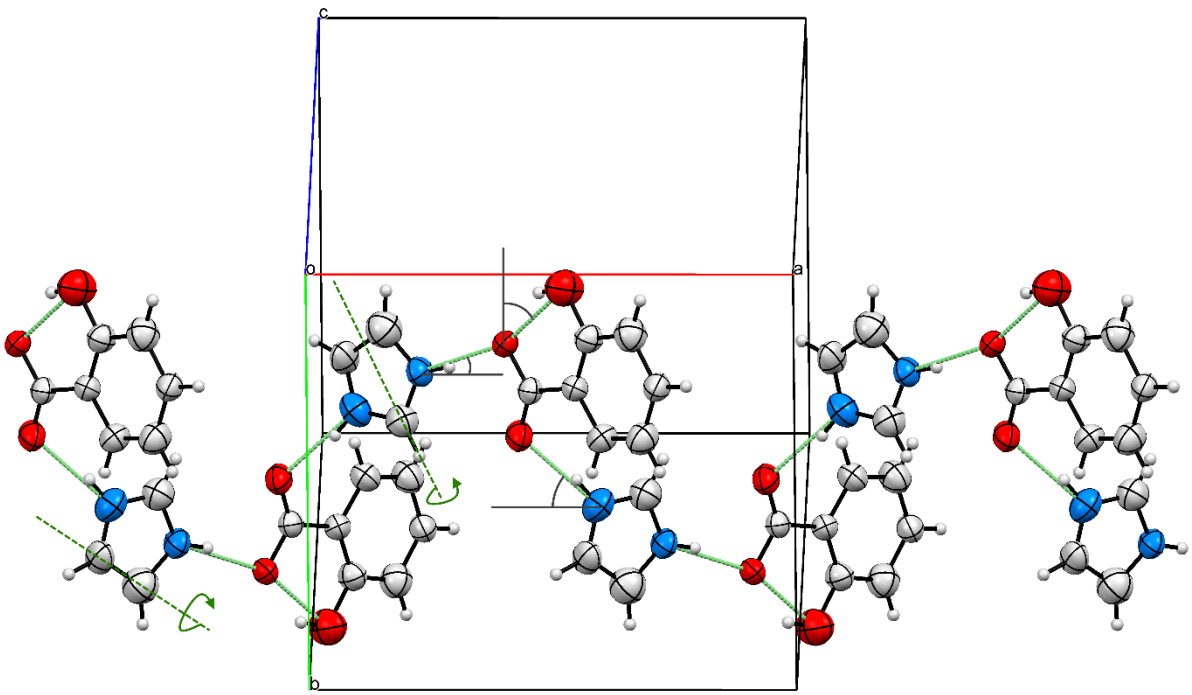

Figure S10. Crystal structure of imidazolium salicylate. The dotted lines denote the axes where the imidazolium ion rotates in the crystal.

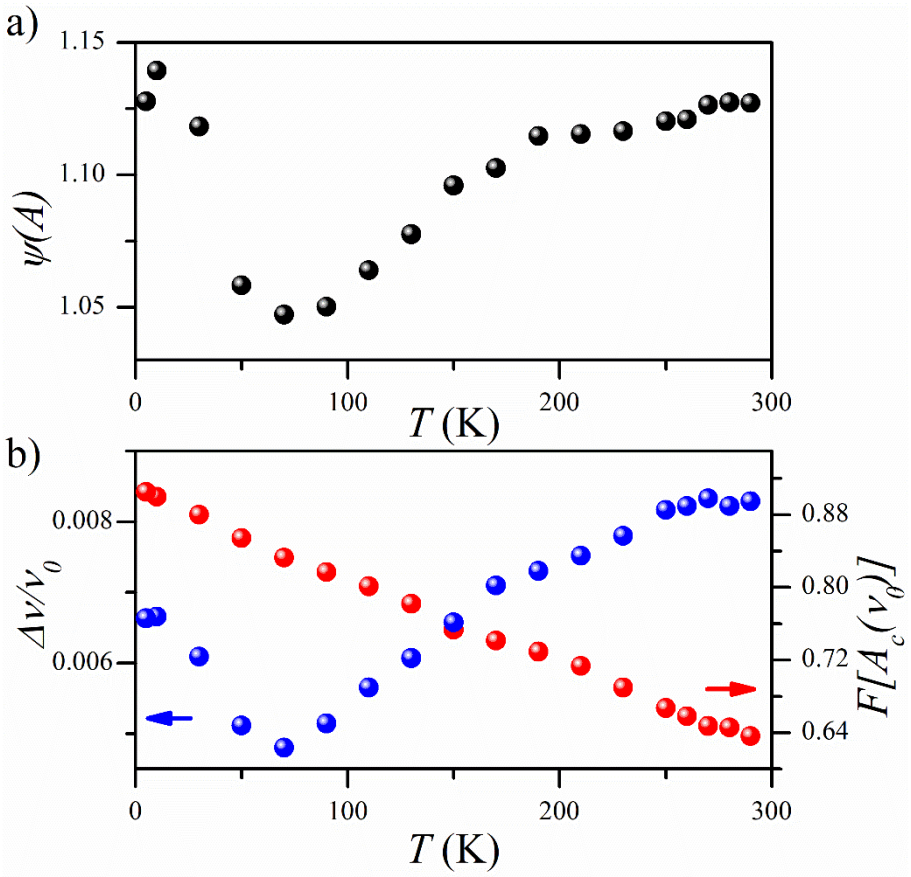

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Table S1. Crystal data, data collection, and structure refinement for **SalImi** at different temperatures at atmospheric pressure

Crystal data					
Chemical formula	$C_{10}H_{10}N_2O_3$	$C_{10}H_{10}N_2O_3$	$C_{10}H_{10}N_2O_3$	$C_{10}H_{10}N_2O_3$	$C_{10}H_{10}N_2O_3$
M_r	206.20	206.20	206.20	206.20	206.20
Crystal system, space group			Orthorhombic, *Pbca*		
Temperatur (K)	100.0(1)	130.0(1)	180.0(1)	240.0(1)	300.0(1)
Unit cell parameters					
a (Å)	11.0676(5)	11.0905(6)	11.1043(5)	11.0988(6)	11.0777(11)
b (Å)	11.0227(5)	10.9922(5)	10.9664(5)	10.9361(5)	10.9375(9)
c (Å)	16.1520(7)	16.1833(8)	16.3069(9)	16.4701(9)	16.6880(15)
α, β, γ (º)	90 ,90, 90	90, 90, 90	90, 90, 90	90, 90, 90	90, 90, 90
V (Å^3)	1970.45(15)	1972.89(16)	1985.76(17)	1999.10(18)	2022.0(3)
Z	8	8	8	8	8
F(000)	864	864	864	864	864
D_x (Mg m^{-3})	1.390	1.388	1.379	1.370	1.355
Radiation type, λ(Å)			Mo *Kα*, 0.71073		
μ (mm^{-1})	0.105	0.105	0.104	0.103	0.102
Crystal shape			Block		
Color			Colourless		
Crystal size (mm)			0.30 x 0.26 x 0.13		
Data collection					
Diffractometer	SuperNova, Dual Mo, Atlas	SuperNova, Dual Mo, Atlas	SuperNova, Dual Mo, Atlas	SuperNova, Dual Mo, Atlas	SuperNova, Dual Mo, Atlas
Absorption correction	Multi-scan (CrysAlis PRO). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.				
T_{min}, T_{max}	0.700, 1.000	0.628, 1.000	0.640, 1.000	0.626, 1.000	0.582, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16383, 2561, 2214	16447, 2578, 2173	16741, 2567, 2058	16879, 2584, 1913	15447, 2617, 1775
Measurement method			ω scans		
R_{int}	0.0274	0.0360	0.0340	0.0334	0.0375
θ_{max}, θ_{min} (º)	29.51, 2.90	29.60, 2.52	29.64, 2.89	29.67, 2.89	29.66, 2.44
Structure refinement					
R [$F^2 \geq 2\sigma(F^2)$], $wR(F^2)$, S	0.0400, 0.1033, 1.080	0.0450, 0.1222, 1.087,	0.0465, 0.1153, 1.077	0.0493, 0.1362, 1.074	0.0524, 0.1418, 1.067
No. of reflections	2561	2578	2567	2584	2617
No. of parameters	148	148	149	149	149
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.291, –0.267	0.261, –0.313	0.364, –0.182	0.323, –0.181	0.249, –0.219
Extinction correction	$F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$				
Extinction coefficient	–	–	0.0069(9)	0.0075(11)	0.0121(14)

Table S2. Crystal data, data collection, and structure refinement for **SalImi** at different pressures at room temperature (T=293.02 K).

Chemical formula	$C_{10}H_9N_2O_3$	$C_{10}H_9N_2O_3$	$C_{10}H_9N_2O_3$	$C_{10}H_9N_2O_3$	$C_{10}H_9N_2O_3$
Formula weight	206.19	206.19	206.19	206.19	206.19
Pressure (GPa)	0.16	0.95	1.30	1.67	2.27
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Pbca*	*Pbca*	*Pbca*	*Pbca*	*Pbca*
Unit cell parameters (Å, º)	a=11.2640(13) b=10.812(11) c=16.025(2)	a=11.4739(8) b=10.652(7) c=15.1725(13)	a=11.5502(8) b=10.596(7) c=14.8160(13)	a=11.562(3) b=10.656(19) c=14.409(3)	a=11.540(5) b=10.49(4) c=14.153(8)
Volume ($Å^3$)	1952(2)	1854.4(12)	1813.3(12)	1775(3)	1713(7)
Z	8	8	8	8	8
F(000)	864.0	864.0	864.0	864.0	864.0
Calculated density (g cm^{-3})	1.404	1.477	1.511	1.543	1.599
Absorption coefficient (mm^{-1})	0.106	0.111	0.114	0.116	0.120
Crystal dimensions [mm]			0.20 x 0.18 x 0.13		
Θ Range for data collection (º)	4.625 to 26.634	4.773to 24.757	4.841 to 21.998	4.495 to 19.579	4.956 to 27.269
Max./Min. indices	h:-13→13 k:-4→4 l:-19→19	h:-14→14 k:-4→4 l:-18→18	h:-14→14 k:-4→4 l:-18→18	h:-14→14 k:-4→4 l:-17→17	h:-14→14 k:-3→3 l:-17→17
Ref. collected/unique	7165/792	7603/744	7442/732	6634/612	5289/576
Observed reflections [$I \geq 2\sigma(I)$]	1007	1207	1257	702	581
R_{int}	0.1218	0.0830	0.0787	0.1062	0.1165
Parameters	138	137	137	137	118
final R indices [I>2$\sigma(I)$]	R_1=0.0743 wR_2=0.1879	R_1=0.0535 wR_2=0.1264	R_1=0.0553 wR_2=0.1273	R_1=0.0743 wR_2=0.1963	R_1=0.0987 wR_2=0.2377
R indices (all data)	R_1=0.1702 wR_2=0.2554	R_1=0.1336 wR_2=0.1688	R_1=0.1407 wR_2=0.1712	R_1=0.2221 wR_2=0.2991	R_1=0.2370 wR_2=0.3536
goodness of fit of F^2	1.012	1.014	1.018	1.018	1.048
Largest diff. peak and hole	0.13/-0.14	0.12/-0.17	0.13/-0.16	0.14/-0.16	0.21/-0.18

Table S3. Cell parameters (Å, °) for **SalImi** at different temperatures (K).

Temperature	*a*	*b*	*c*	*α*	*β*	*γ*	*V*
100	11.0676(5)	11.0227(5)	16.1520(7)	90.00	90.00	90.00	1970.46(15)
130	11.0905(6)	10.9922(5)	16.1833(8)	90.00	90.00	90.00	1972.89(16)
180	11.1043(5)	10.9664(5)	16.3069(9)	90.00	90.00	90.00	1985.76(17)
240	11.0988(6)	10.9361(5)	16.4701(9)	90.00	90.00	90.00	1999.10(18)
300	11.0777(11)	10.9375(9)	16.6880(15)	90.00	90.00	90.00	2022.0(3)

Table S4. Cell parameters (Å, °) for **SalImi** at different pressures (GPa).

Pressure	*a*	*b*	*c*	*α*	*β*	*γ*	*V*
0.16	11.2640(13)	10.812(11)	16.025(2)	90.00	90.00	90.00	1952(2)
0.95	11.4739(8)	10.652(7)	15.1725(13)	90.00	90.00	90.00	1854.4(12)
1.30	11.5502(8)	10.596(7)	14.8160(13)	90.00	90.00	90.00	1813.3(12)
1.67	11.562(3)	10.656(19)	14.409(3)	90.00	90.00	90.00	1775(3)
2.27	11.540(5)	10.49(4)	14.153(8)	90.00	90.00	90.00	1713(7)

Table S5. The second and third-order Birch-Murnaghan coefficient of volume under pressure for SalImi: B_0 (GPa) - the bulk modulus, B_0' the bulk modulus pressure derivative, V_0 (Å^3) the unit cell volume at ambient conditions, and with σ their standard errors.

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	B_0'	σB_0'
2nd	11.7	0.5	1985.4	7.7	4.0	0
3nd	14.5	0.3	1973.1	1.5	1.8	0.2

Table S6. Hydrogen-bonds and C–H···*Cg* interactions (Å, °) in the crystal structure of **SalImi** at different temperatures.

Temperature (K)	*D*—H···*A*	*D*–H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*–H···*A* (º)
100	N1a–H1a···O9b N2a–H2a···O8b^{i} O10b–H10b··O9b C3a–H3aa···O10b^{ii}	0.93(2)	1.77(2)	2.6903(13)	174.6(18)
		0.95(2)	1.74(2)	2.6779(13)	165.7(19)
		0.98(2)	1.61(2)	2.5300(13)	155(2)
		0.95	2.41	3.2545(16)	148
130		0.93(2)	1.77(2)	2.6950(15)	173(2)
		0.93(2)	1.77(2)	2.6798(15)	166(2)
		0.96(2)	1.62(2)	2.5285(14)	156(2)
		0.95	2.42	3.2537(18)	147
180		0.92(2)	1.80(2)	2.7079(16)	172(2)
		0.93(2)	1.78(2)	2.6873(17)	167(2)
		0.98(2)	1.60(2)	2.5275(16)	156(2)
		0.95	2.44	3.266(2)	145
240		0.92(3)	1.81(3)	2.7199(19)	171(2)
		0.93(2)	1.77(2)	2.692(2)	170(2)
		1.01(2)	1.56(2)	2.5245(19)	157(2)
		0.94	2.47	3.278(2)	144
300		0.94(3)	1.80(3)	2.731(2)	169(2)
		0.92(3)	1.79(3)	2.701(2)	170(3)
		1.05(3)	1.54(3)	2.525(2)	156(3)
		0.93	2.51	3.303(3)	143
Temperature (K)	*C*–H···*Cg*	C–H (Å)	*H*···*Cg* (Å)	C···*Cg* (Å)	C–H···*Cg* (º)
100	C2a–H2aa···*Cg*1^{iii}	0.95	2.68	3.5667(14)	156
130		0.95	2.69	3.5777(16)	156
180		0.95	2.72	3.6067(18)	156
240		0.94	2.77	3.645(2)	156
300		0.93	2.82	3.689(2)	156

Symmetry codes: (i) $-1/2+x,3/2-y,1-z$; (ii) $-1/2+x,1/2-y,1-z$; (iii) $3/2-x,1-y,1/2+z$. *Cg*1 is phenyl ring centroid.

Table S7. Hydrogen bond geometry (Å, °) for **SalImi** at different pressures.

Pressure (GPa)	*D*–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
0.16	N1a–H1a···O9b N2a–H2a···O8b^{i} O10b–H10b··O9b C3a–H3aa···O10b^{ii}	0.86(1)	1.89(1)	2.737(13)	169.9(12)
		0.86(1)	1.84(1)	2.700(20)	174.2(8)
		0.82(1)	1.85(1)	2.544(15)	141.3(10)
		0.93(2)	2.35(1)	3.120(30)	140.2(7)
0.95		0.86(1)	1.86(1)	2.698(9)	168.0(8)
		0.86(1)	1.86(1)	2.711(15)	168.7(7)
		0.82(1)	1.81(1)	2.527(11)	144.7(8)
		0.93(2)	2.38(1)	3.138(19)	138.9(5)
1.30		0.86(1)	1.86(1)	2.697(10)	163.2(9)
		0.86(1)	1.84(1)	2.680(17)	166.6(7)
		0.82(1)	1.85(1)	2.548(9)	142.4(8)
		0.93(2)	2.33(1)	3.061(21)	135.3(6)
1.67		0.86(1)	1.86(1)	2.685(18)	161.2(15)
		0.86(2)	1.85(1)	2.682(31)	163.5(11)
		0.82(1)	1.90(1)	2.561(20)	136.5(13)
		0.93(3)	2.28(1)	3.011(42)	135.2(12)
2.27		0.86(1)	1.88(1)	2.701(18)	159.4(16)
		0.86(3)	1.83(1)	2.663(33)	164.5(12)
		0.82(1)	1.81(1)	2.513(21)	143.5(13)
		0.93(4)	2.28(1)	2.990(40)	132.9(12)

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

Table S8. SalImi QTAiM parameters (in atomic unit) as a function of temperature corresponding to the H···O bond critical point (BCPs), the electron density at BCP ρ_{BCP}; Laplacian of electron density at BCP, $\Delta\rho_{BCP}$; total electron energy density at BCP, H_{BCP} and the components of the H_{BCP}: kinetic electron energy density, G_{BCP}; potential electron energy density, V_{BCP}, the hydrogen bond energy, E_{HB} (kcal·mol^{-1}).

	T (K)	ρ_{BCP}	Δ_{BCP}	G_{BCP}	V_{BCP}	H_{BCP}	E_{HB}
O10b–H10b···O9b	100	0.0590	0.1655	0.0521	-0.0628	-0.0107	-19.69
	130	0.0574	0.1668	0.0513	-0.0609	-0.0096	-19.12
	180	0.0613	0.1659	0.0535	-0.0656	-0.0121	-20.58
	240	0.0631	0.1648	0.0544	-0.0676	-0.0132	-21.22
	300	0.0663	0.1619	0.0559	-0.0713	-0.0154	-22.37
N1a–H1a···O9b	100	0.0394	0.1333	0.0345	-0.0358	-0.0012	-11.22
	130	0.0396	0.1317	0.0344	-0.0358	-0.0014	-11.23
	180	0.0370	0.1279	0.0324	-0.0328	-0.0004	-10.29
	240	0.0352	0.1241	0.0308	-0.0306	0.0002	-9.58
	300	0.0363	0.1218	0.0309	-0.0314	-0.0005	-9.85
N2a–H2a···O8b^{i}	100	0.0396	0.1436	0.0365	-0.0370	-0.0006	-11.62
	130	0.0378	0.1423	0.0353	-0.0350	0.0003	-10.99
	180	0.0367	0.1400	0.0344	-0.0337	0.0007	-10.57
	240	0.0372	0.1403	0.0347	-0.0343	-0.0004	-10.75
	300	0.0344	0.1362	0.0325	-0.0310	0.0015	-9.74

Table S9. SalImi QTAiM parameters (in atomic unit) as a function of pressure corresponding to the H···O bond critical point (BCPs), the electron density at BCP ρ_{BCP}; Laplacian of electron density at BCP, $\Delta^2\rho_{BCP}$; total electron energy density at BCP, H_{BCP} and the components of the H_{BCP}: kinetic electron energy density, G_{BCP}; potential electron energy density, V_{BCP}, the hydrogen bond energy, E_{HB}.

	p (GPa)	ρ_{BCP}	Δ_{BCP}	G_{BCP}	V_{BCP}	H_{BCP}	E_{HB}
O10b–H10b···O9b	0.16	0.0354	0.1457	0.0353	-0.0341	0.0012	-10.71
	0.95	0.0357	0.1456	0.0354	-0.0344	0.0009	-10.79
	1.30	0.0347	0.1430	0.0345	-0.0332	0.0013	-10.41
	1.67	0.0315	0.1308	0.0308	-0.0289	0.0019	-9.07
	2.27	0.0315	0.1353	0.0316	-0.0294	0.0022	-9.22
N1a–H1a···O9b	0.16	0.0305	0.1152	0.0271	-0.0254	0.0017	-7.96
	0.95	0.0327	0.1251	0.0297	-0.0282	0.0015	-8.85
	1.30	0.0326	0.1243	0.0295	-0.0279	0.0015	-8.78
	1.67	0.0325	0.1288	0.0303	-0.0284	0.0019	-8.91
	2.27	0.0370	0.1401	0.0344	-0.0337	0.0006	-10.58
N2a–H2a···O8b^{i}	0.16	0.0315	0.1354	0.0309	-0.0281	0.0029	-8.82
	0.95	0.0307	0.1291	0.0295	-0.0267	0.0028	-8.36
	1.30	0.0322	0.1359	0.0313	-0.0287	0.0027	-9.00
	1.67	0.0322	0.1317	0.0306	-0.0283	0.0023	-8.87
	2.27	0.0359	0.1516	0.0359	-0.0339	0.0020	-10.64

Table S10. Parameters of the helicoid: a_h (semi-major axis), b_h (semi-minor axis), Sh_h (helix pitch), c_h (focal length of the ellipse), e_h (eccentricity of the ellipse), l_h (circumference of the ellipse), and S_h (area of the ellipse).

		$2a_h$ (Å)	a_h (Å)	$2b_h$ (Å)	b_h (Å)	Sh_h (Å)	c_h (Å)	e_h	S_h (Å^2)	l_h (Å)
T (K)	300	6.73	3.37	3.09	1.55	11.07	2.99	0.89	16.36	15.96
	240	6.73	3.37	3.05	1.52	11.09	3.00	0.89	16.11	15.91
	180	6.74	3.37	3.02	1.51	11.12	3.01	0.89	15.99	15.89
	130	6.75	3.37	2.99	1.50	11.13	3.02	0.90	15.85	15.87
	100	6.76	3.38	2.98	1.49	11.06	3.03	0.90	15.85	15.88
p (GPa)	0.16	6.65	3.33	3.03	1.51	11.28	2.96	0.89	15.82	15.74
	0.95	6.57	3.28	2.88	1.44	11.53	2.95	0.90	14.85	15.40
	1.3	6.57	3.28	2.83	1.42	11.58	2.96	0.90	14.60	15.35
	1.67	6.57	3.29	2.77	1.39	11.65	2.98	0.91	14.29	15.28
	2.27	6.53	3.27	2.72	1.36	11.67	2.97	0.91	13.96	15.15

Table S11. The assignment of the selected vibrational bands observed in FT-IR and Raman spectra of **SalImi**.

ν FT-IR (cm^{-1})	ν Raman (cm^{-1})	Assignment	Literature	ν calc.* (cm^{-1})
3159	3165	ν(N–H)	[1]	3180
3151	3152	ν(N–H)	[1]	3168
1626	1630	ν(C=C)	[1]	1644
1572	1567	ν_{asym}(COO)	[1, 6]	1601
	1524	ν(C–N)	[1]	1509
1486	1480	ν(C–COO)	[1, 6]	1559
1462	1454	ring mode + δ(CNH)	[1]	1460
1388		ν_{sym}(COO)	[1]	1354
1346		ν(C–OH)	[1]	1323
905	912	γ(CCH)	[1]	908
890	896	δ(NCN)	[1]	892
859	855	γ(CNH)	[1]	862
808	807	δ(CCN)	[1]	780
757	759	δ(CCH)	[1]	751

*calculated normal modes of imidazolium and acid ions using ωB97XD/6-311++G(d,p) method; scaling factor of 0.97 was used.

Table S12. The assignment of the selected bands observed in Raman spectra in the phonon spectral range of **SalImi**.

ν Raman (cm^{-1})	Assignment	Literature
136	ν(N^+–H···O^-)	[2-5]
99	ν(N^+–H···O^-)	[2-5]
53	γ(N^+–H···O^-)	[2-5]
40	γ(N^+–H···O^-)	[2-5]

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Table S13. Lengths and angles of the bonds in the imidazole ion as a function of the temperature. Note: The atomic labeling scheme is shown in Figure S2.

	100 K	130 K[1]	180 K	240 K	300 K
Bond Lengths (Å)					
N1a-C1a	1.324	1.323	1.316	1.311	1.306
N2a-C1a	1.329	1.327	1.324	1.319	1.319
N1a-C3a	1.371	1.366	1.358	1.349	1.342
N2a-C2a	1.367	1.361	1.353	1.344	1.342
C2a-C3a	1.347	1.340	1.329	1.317	1.308
Angles (°)					
N1a-C1a-N2a	108.5	108.4	108.3	108.3	108.2
C1a-N1a-C3a	108.6	108.6	108.6	108.5	108.5
C1a-N2a-C2a	108.6	108.5	108.3	108.0	107.8
N1a-C3a-C2a	107.0	107.1	107.1	107.1	107.4
N2a-C2a-C3a	107.2	107.4	107.6	108.0	108.1

Table S14. Lengths and angles of the bonds in the imidazole ion as a function of the pressure. Note: The atomic labeling scheme is shown in Figure S2.

	0.16 GPa	0.95 GPa	1.3 GPa	1.67 GPa	2.27 GPa
Bond Lengths (Å)					
N1a-C1a	1.392	1.327	1.296	1.299	1.299
N2a-C1a	1.341	1.289	1.297	1.287	1.299
N1a-C3a	1.398	1.361	1.383	1.416	1.298
N2aC2a	1.277	1.258	1.317	1.342	1.296
C2a-C3a	1.402	1.364	1.348	1.352	1.298
		Angles (°)			
N1a-C1a-N2a	100.2	105.9	108.5	108.3	107.9
C1a-N1a-C3a	115.6	109.6	110.7	111.8	107.9
C1a-N2a-C2a	113.1	112.2	108.1	108.2	108.1
N1a-C3a-C2a	97.5	103.0	101.7	99.7	108.1
N2a-C2a-C3a	113.1	109.2	111.0	111.9	107.9