Supplementary Materials

Structure-property relationships in hybrid: (C₃H₅N₂)₃[Sb₂I₉] and (C₃H₅N₂)₃[Bi₂I₉] isomorphs

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TABLE OF CONTENTS:

1. X-ray characterization
2. Dielectric properties
3. Optical properties
4. Proton magnetic resonance studies (¹H NMR)
5. Vibrational properties
Figure S1. The numbering scheme for Table S1 and ellipsoid representation of the imidazolium A and B, respectively, in the orthorhombic phase II

Table S1. Selected hydrogen-bond parameters for ImIA and ImIB at RT. Bonds involving imidazolium A (yellow) and B (grey) are distinguished and highlighted by the colours of the background.

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<th>Type of cation</th>
<th>$D$—$H$···$A$</th>
<th>$D$—$H$ (Å)</th>
<th>$H$···$A$ (Å)</th>
<th>$D$···$A$ (Å)</th>
<th>$D$—$H$···$A$ (°)</th>
<th>Symmetry code(s)</th>
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<td>2.72</td>
<td>3.30 (4)</td>
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<td>A</td>
<td>i, x+1/2, y+1/2, z+1/2</td>
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<td>II, x, y, -z+1/2</td>
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<td>C8—H8···I2</td>
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<td>3.04</td>
<td>3.76 (4)</td>
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Symmetry code(s): i, x+1/2, y+1/2, z; ii, -x+1/2, -y+1/2, -z+1; iii, -x+1/2, -y+1/2, -z+1; iv, x, -y, z+1/2; I, -x+1/2, y+1/2, z+1/2; II, -x+1/2, -y+1/2, -z+1; III, x+1/2, y+1/2, z+1; IV, x, y, z+1/2.
Part 2
In Figure S2 one can see that below 90 K a clear deviation of $\varepsilon$ from the Cole-Cole plot at frequencies above ca. 0.5 MHz takes place. This seems to indicate another dispersion in the megahertz frequency region at low temperatures. Nevertheless, these two relaxators (low frequency (1) which is fundamental for this compound and expected higher frequency one (2)) are overlapped thus it was impossible to elaborate the dielectric parameters for (2).

Figure S2. Cole-Cole plots at selected temperatures in ImIB (phase III).

Figure S3 Temperature dependence of macroscopic relaxation time $\tau$ versus temperature and $\ln(\tau)$ versus reciprocal temperature for low frequency relaxator (1) for ImIB.
Figures S4 (a) and (b) and Figure 5 clearly show the divergence of the complex dielectric permittivity between 350 and 220 K which is mainly due to the conductivity phenomena. The dielectric characteristics presented in Figure S4 (b) do not indicate any relaxation process in ImIA in the analyzed frequency region.
Figure S5: Evolution of the domain structure in ImIB in one cooling cycle.
Part 4

The $T_{1(H-H)}$ relaxation rate is given as a combination of spectral densities:\textsuperscript{1-5}

$$
\frac{1}{T_{1(H-H)}} = C\left(\frac{\tau}{1 + \omega_H^2 \tau^2} + \frac{4\tau}{1 + 4\omega_H^2 \tau^2}\right),
$$

(eq. S1)

where $\omega_H$ is the Larmor proton frequency and $C$ is the relaxation constant:

$$
C = (a_{HH}^{DD})^2 = \left(\frac{\gamma^H \gamma^H \hbar}{r_{H-H}^3}\right)^2.
$$

The other relaxation rates can be obtained from well-known formulas for the spin–lattice relaxation rate of two different spins:\textsuperscript{1-3}

$$
\frac{1}{T_{1(H-X)}} = \frac{2}{3}(a_{HX}^{DD})^2 l_x (l_x + 1) \left(\frac{\tau}{1 + (\omega_H - \omega_X)^2 \tau^2} + \frac{3\tau}{1 + \omega_H^2 \tau^2} + \frac{6\tau}{1 + (\omega_H + \omega_X)^2 \tau^2}\right),
$$

(eq. S2)

where: $\omega_X$, ($X = N$, Sb or Bi, I) are Larmor frequencies of the nuclei in the given compound, $a_{HX}^{DD}$ are the dipole–dipole constants, while $l_N = 1$, $l_{Sb(121)} = 5/2$, $l_{Sb(123)} = 7/2$, $l_{Br} = 3/2$. $l_l = 5/2$. For simplicity, we assumed the simplest possible form of spectral densities functions with a single exponential dependence of the correlation time versus temperature according to Arrhenius law: $\tau = \tau_0 \exp (E_a/RT)$, where $E_a$ is activation energy.

**Table S2** Selected parameters (obtained from eqs. 6 and S1) of three different types of imidazolium cations. Labeling of the cations concerns the lowest temperature phase (III).

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<th>parameter</th>
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<th>ImIA</th>
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<td>$E_a$</td>
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<td>1.25 kcal/mol</td>
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<td>$\tau_0$</td>
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<td>$C_1$</td>
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<td>2</td>
<td>$E_a$</td>
<td>2.82 kcal/mol</td>
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<td></td>
<td>$\tau_0$</td>
<td>6.07 $10^{-14}$s</td>
<td>3.77 $10^{-14}$s</td>
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<tr>
<td></td>
<td>$C_2$</td>
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<td>3</td>
<td>$E_a$</td>
<td>5.21 kcal/mol</td>
<td>5.4 kcal/mol</td>
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<td></td>
<td>$\tau_0$</td>
<td>9.91 $10^{-14}$s</td>
<td>9.94 $10^{-14}$s</td>
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<td></td>
<td>$C_3$</td>
<td>1.05 $10^8$s$^{-2}$</td>
<td>1.17 $10^8$s$^{-2}$</td>
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</table>
Figure S6. Temperature dependence of second moment of $^1$H NMR line of ImIA (blue) and ImIB (red).

References:
Part 5

The infrared spectra of polycrystalline \((\text{C}_3\text{H}_5\text{N}_2)_3[\text{M}_2\text{I}_9]\), \((\text{M} = \text{Sb}, \text{Bi})\) in the wavenumbers range between 4000 and 500 \text{cm}^{-1} \text{ at } 300 \text{ K (phase II) and 413 K (phase I)}, and Raman spectra (300 K) are presented in Figures S7-S10. The IR spectra in the frequency range 3000–2800, 1500–1350, 750–700 \text{ cm}^{-1} are shown as dotted lines as Nujol bands appear in these regions. To cover these areas infrared spectrum in Fluorolube mull at 300 K was measured. Tentative assignments of the observed bands (Table S3) were based on the comparison with imidazole amine.6-11

![Figure S7.](image)

**Figure S7.** (a) Infrared spectra of powdered ImIA (blue) and ImIB (red) samples in Nujol and Fluorolube (at 300 and 11 K (only for ImIB)); (b) Raman spectra at 300 K.

**Experimental details:** Powder FT-Raman spectra were recorded with FRA-106 attachment to the Bruker IFS-88 using Nd:YAG diode pump laser. The measurements were performed over the wavenumber range 3500–80 \text{ cm}^{-1} at room temperature with a resolution better than 2 \text{ cm}^{-1}.

**References:**
Formal classifications of the fundamental modes for ImIA and ImIB

These two crystals posses two phases; hexagonal (phase I) ($P6_3/mmc = D_{2h}^4$, $Z = 2$) and orthorhombic (phase II) ($Cmcn = D_{2h}^{17}$, $Z = 4$). According to the x-ray data, the $[\text{Sb}_2\text{I}_9]^{3-}$ anions occupy the $D_{3h}$ sites in the case of phase I and $C_{2v}$ site in the phase II. In both phases, there are two independent types, A and B, of the imidazolium cations. In the high –temperature phase (I), the A type cations occupy the positions close to $C_{3v}(4)$ sites, whereas the B type cations occupy the positions close to the $D_{3h}(2)$ sites. However, in each case, for both cations there exists a 3-fold disorder, and only one of these positions is occupied by each cation, respectively. Thus, for the A –type cations each of them may occupy one position with the approximate symmetry $C_s$ (the plane symmetry is perpendicular to the plane of heavy atoms), whereas, the B-type cations occupy one of the three possible positions of $C_s$ symmetry, however in this case all atoms lie in the symmetry plane ($C_s$).

In phase II, the B cations become ordered and occupy the $C_{2v}$ site symmetry. The A type cations still remain disordered and occupy one of two possible positions related by the $C_s$ plane being perpendicular to the a-axis. The highest symmetry of the imidazolium cation is $C_{2v}$ and their normal modes may transform as follows: $(9\ A_1(//z, xx,yy,zz) + 3A_2 i, xy) + 8B_1 (//x, zy) + 4 B_2 (//y, yz))$. For the Cs symmetry its modes are either $17 A' (//x, //y, xx, yy, zz, xy) + 7 A''(//z, yz, zx)$, for all atoms lying the symmetry plane, or $13 A' (//x, //y, yy,zz, xy) + 11A'' (//z, yz, zx)$ for only two atoms (C-H) lying in that plane. Of course, it is also possible that both type of these cations are of $C_s$ symmetry and all their internal modes (24) are of A type only.

As it follows from the X-ray data, the iodoantimonate(III) anions ($[\text{Sb}_2\text{I}_9]^{3-}$) are ordered in both phases. They have a face-sharing biooctahedra shape. They occupy the $D_{3h}$ (3m.) site in the high-temperature phase I. They conserve the face-sharing biooctahedral shape in phase II, although their symmetry changes to $C_{2v}$ symmetry. The $x\_y$ plane remains and it is perpendicular to the c-axis; it contains I(1) and two I(2) atoms. The twofold axis is parallel to the b axis and only one atom I(1) lies on it. The second mirror plane is perpendicular to the a-axis and it contains two Sb atoms, I1 and two I4 atoms. The internal modes of the iodoantimonate(III) anions of $D_{3h}$ site symmetry can be classified as $4A_1(xx+yy,zz) + A_2' + 5E' (X,Y; xx-yy,xy) + A_1'' + 3A_2''(Z) +4E''(yz,zx)$, among which 8 modes ($5E' + 3A_2''$) are IR active and $13 (4A_1' + 5E' + 4E'')$ are Raman active. The internal modes for the iodoantimonate(III) anions of $C_{2v}$ site symmetry can be classified as: $9A_1 (Z, xx,yy, zz) + 5A_2 (xy) + 6B_1 (X, zx) + 7 B_2 (Y, yz)$; all of them are allowed in Raman (27 modes) and only 22 are allowed in the IR spectra. Thus, one can expect significant differences between the vibrational spectra (IR and Raman) of the title crystal measured in these two phases.
Figure S8. (a) Infrared spectra between 895 and 925 cm$^{-1}$ of the ImIB as functions of temperature, (b) plot of the wavenumber $\beta$(R), $\beta$(CH) mode frequencies of ImIB as a function of temperature (R-ring).

Figure S9. (a) The infrared spectra between 1030 and 1110 cm$^{-1}$ of the ImIB as functions of temperature, (b) plot of the $\nu$(R) $\delta$(CH) mode frequencies of ImIB as a function of temperature.
Figure S10. (a) The infrared spectra between 1140 and 1310 cm\(^{-1}\) of the ImIB as a function of temperature, (b) plot of the Ring breathing, \(\nu(R)\), \(\beta(CH)\) mode frequencies of ImIB as a function of temperature.

Figure S11. (a) The infrared spectra between 3000 and 3400 cm\(^{-1}\) of the ImIB as functions of temperature, (b) plot of the \(\nu(NH)\) mode frequencies of ImIB as a function of temperature.
Table S4.
Wavenumbers (cm\(^{-1}\)) and relative intensities of the bands observed in the Infrared and Raman spectra of ImIB and Raman at 293 K) and ImIA (IR and Raman at 293 K). IR spectra as functions of temperature were measured for the emulsion in Nujol in between CsI windows.

<table>
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<th>IR</th>
<th>Raman</th>
<th>Assignments(^{11})</th>
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<td><strong>ImIA</strong></td>
<td><strong>ImIB</strong></td>
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<tr>
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\(\nu(R)+\beta(CH)+\beta(NH)\)

\(\nu(R)+\beta(CH)\)

Ring breathing

\(\nu(R)+\delta(CH)\)

\(\nu(R)+\beta(CH)\)
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Legend: vs – very strong; s – strong; m – medium, w – weak, vw – very weak, sh – shoulder; v - stretching; δ - in-plane bending (scissoring); ω - out-of-plane bending (wagging); τ - out-of-plane bending (twisting); β in-plane bending; R – ring.