Reversible Phase Transition with Ultra Large Dielectric Relaxation Behaviors in Succinimide - Lithium (I) Hybrids

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Supporting materials

Figure S1 the colorless block crystal of compound **1**

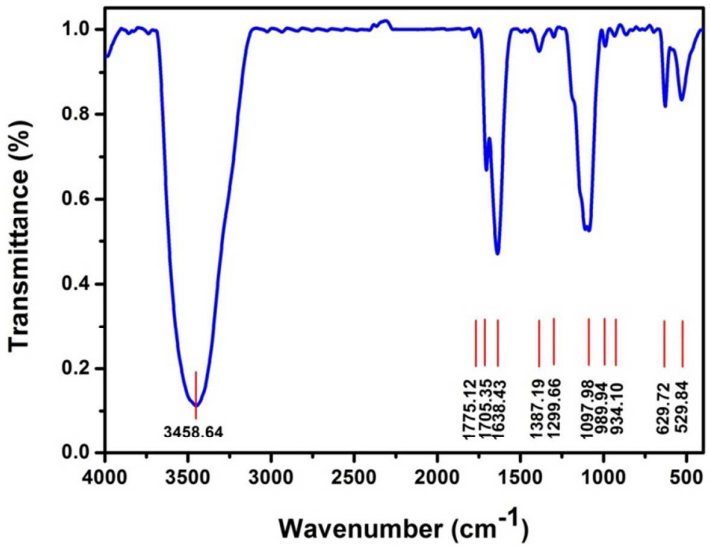


Figure S2 IR spectra of compound 1 at room temperature

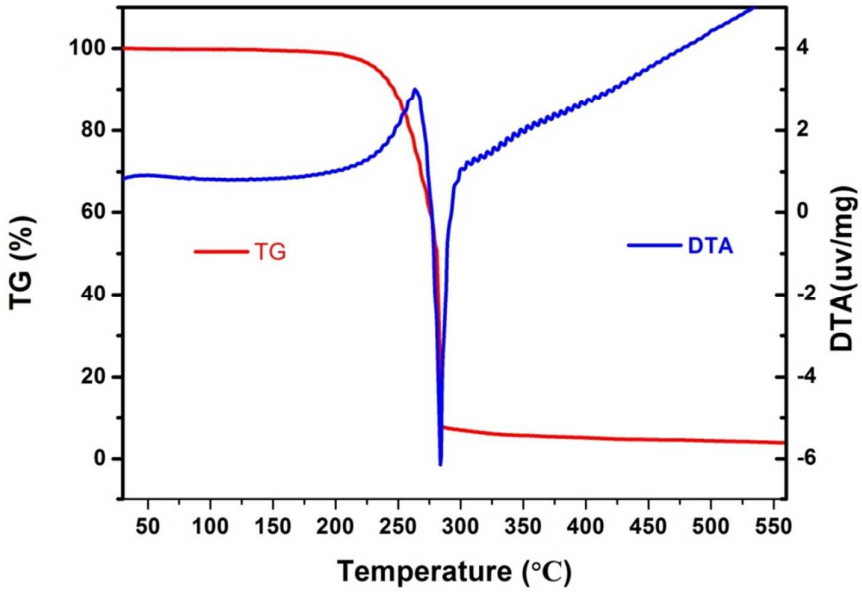


Figure S3 Thermo gravimetric (TG) and Differential Thermal Analysis (DTA) curves of compound **1**

Calculation of *ΔS* and *N*

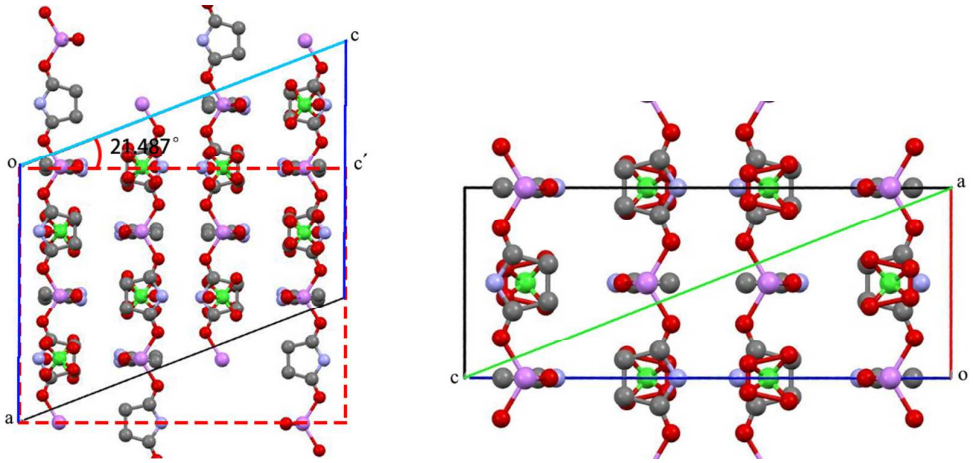
According to the Boltzmann equation, $\Delta S = nR \ln(N)$, where ΔS is the entropy change extracted from the *Cp* data, *n* is the number of guest molecules per mole (n = 1, here), *R* is the gas constant, and *N* is the number of possible orientations for the disordered system. The calculations of ΔS and *N* values on the heating process of **1** are as follows

Calculation of ΔS and N for the cooling cycle in Compound1

$$\Delta S = \int_{T_1}^{T_2} \frac{Q}{T}\, dT$$
$$\approx \frac{\Delta H}{T_C}$$
$$= \frac{1.451\ J \cdot g^{-1} \times 304.5\ g \cdot mol^{-1}}{227.74\ K}$$
$$= 1.94\ J \cdot mol^{-1} \cdot K^{-1}$$
$$\Delta S = R \ln N$$
$$N = \exp\left(\frac{\Delta S}{R}\right) = \exp\left(\frac{1.94\ J \cdot mol^{-1} \cdot K^{-1}}{8.314\ J \cdot mol^{-1} \cdot K^{-1}}\right)$$
$$= 1.26$$

Calculation of ΔS and N for the heating cycle in Compound 1

$$\Delta S = \int_{T_1}^{T_2} \frac{Q}{T}\, dT$$
$$\approx \frac{\Delta H}{T_C}$$
$$= \frac{0.9785\ J \cdot g^{-1} \times 304.5\ g \cdot mol^{-1}}{228.01\ K}$$
$$= 1.31\ J \cdot mol^{-1} \cdot K^{-1}$$
$$\Delta S = R \ln N$$
$$N = \exp\left(\frac{\Delta S}{R}\right) = \exp\left(\frac{1.31\ J \cdot mol^{-1} \cdot K^{-1}}{8.314\ J \cdot mol^{-1} \cdot K^{-1}}\right)$$
$$= 1.17$$



(a) **(b)**

Figure S4 the unit cell unit cell length and *β* angles for (a) **1-LTP** and (b) **1-RTP**

According to the cosine law $a^2=b^2+c^2-2bccosA$ and define of cosine

In **1-LTP** (figure S4a),

oc'=oc×cos∠coc'=oc×cos∠21.487°=21.306 Å×cos∠21.487°=19.825 Å

In **1-RTP** (figure S4b),

$ac=(oa^2+oc^2)^{½}=(7.8674^2+20.046^2)^{½}$Å=21.534 Å

thus, we can obtain

$c_{1\text{-LTP}}$ (21.306 Å) correspond to $a_{1\text{-RTP}}$ -$c_{1\text{-RTP}}$ (21.534 Å)

$c_{1\text{-RTP}}$ (20.046 Å) correspond to $o_{1\text{-LTP}}$ $c_{1\text{-LTP}}$' (19.825 Å)

Table S1 Selected bond lengths (**Å**) and angles for **1-RTP**and**1-LTP**

1-RTP

Bond	Length/Å	Bond Angles	Angle/°
O1-Li1	1.943(3)	O1-Li1-O1^2	118.65(17)
		O1^3-Li1-O1^4	118.65(17)
		O1-Li1-O1^4	105.08(8)
		O1^3-Li1-O1^2	105.08(8)
		O1^3-Li1-O1	105.08(8)
		O1^4-Li1-O1^2	105.08(8)

Asymmetrical codes:^{1}-X,1/2-Y,+Z; ^{2}-1/4-Y,-1/4+X,1/4-Z; ^{3}-X,-1/2-Y,+Z; ^{4}1/4+Y,-1/4-X,1/4-Z;

1-LTP

Bond	Length/Å	Bond	Angle/°
O15-Li1	1.990(13)	O13-Li1-O19	111.5(6)

O16-Li2[1]	1.910(14)	O13-Li1-O15	115.0(6)
O20-Li2[3]	1.909(14)	O13-Li1-O17	104.4(6)
O17-Li1	1.925(13)	O19-Li1-O15	101.3(6)
O19-Li1	1.965(13)	O17-Li1-O19	115.7(6)
O13-Li1	1.916(13)	O17-Li1-O15	109.4(6)
O18-Li2[2]	1.928(14)	O18[5]-Li2-O14	108.7(7)
O14-Li2	1.941(15)	O16[4]-Li2–O14	115.8(8)
		O16[4]-Li2-O18[5]	103.5(6)
		O20[6]-Li2-O16[4]	109.9(7)
		O20[6]-Li2-O14	103.1(6)
		O20[6]-Li2-O18[5]	116.4(8)

Asymmetrical codes: [1]+X,1+Y,+Z; [2]1/2+X,1/2+Y,+Z; [3]-1/2+X,1/2+Y,+Z; [4]+X,-1+Y,+Z; [5]-1/2+X,-1/2+Y,+Z; [6]1/2+X,-1/2+Y,+Z

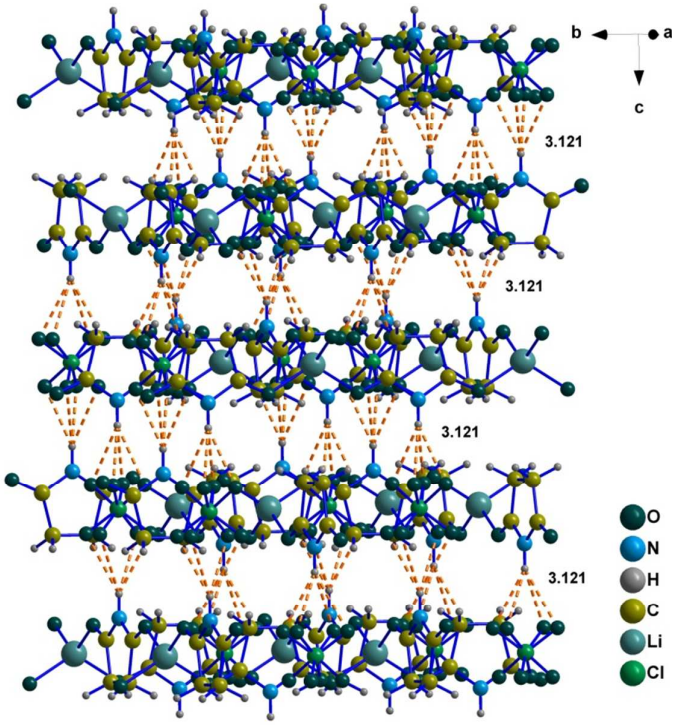


Figure S5 the three dimensional packing structure assembled by hydrogen bond in **1-RTP**

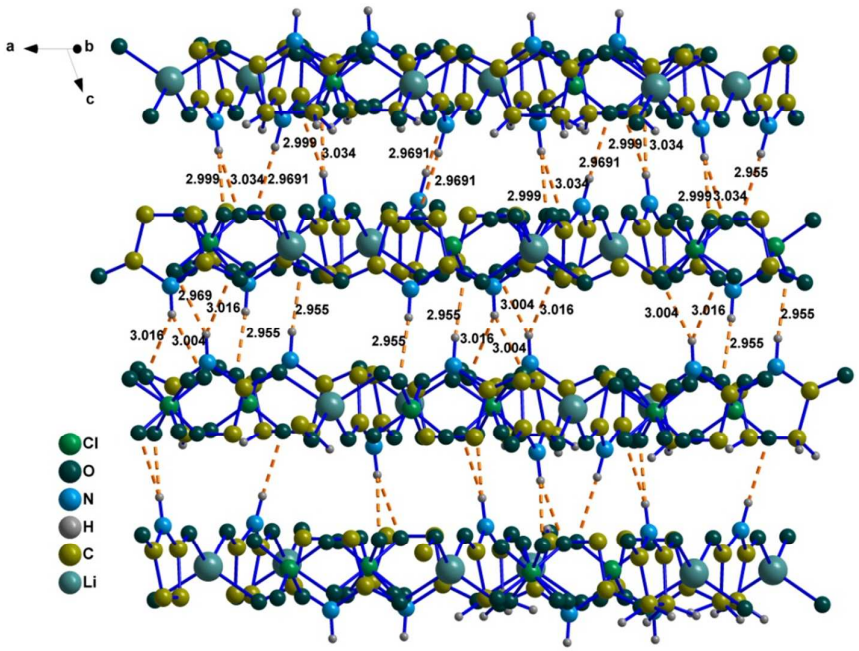


Figure S6 the three-dimensional packing structure assembled by hydrogen bond in **1-LTP**

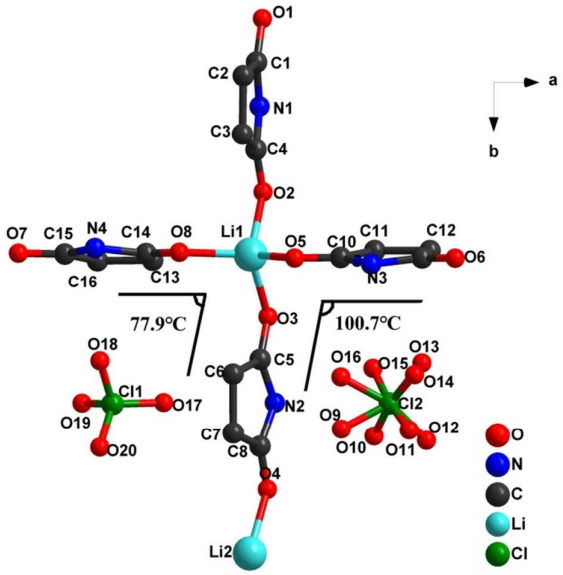


Figure S7 the dihedral angle (78°) between the neighbor pyrrolidine planes in grid **C** in **1-LTP**

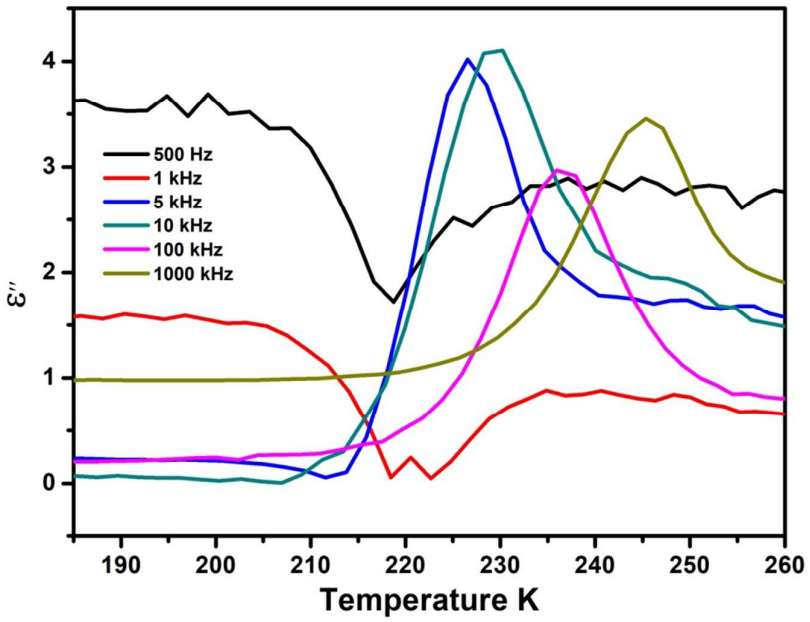


Figure S8 the real part (ε') of the dielectric constant dependence on temperature at different frequency