Supplementary Information

Thermal Energy Storage in A Supramolecular Assembly of $[C_6H_{11}NH_3]^+[CF_3COO]^-$ (C_6H_{11} = Cyclohexyl)

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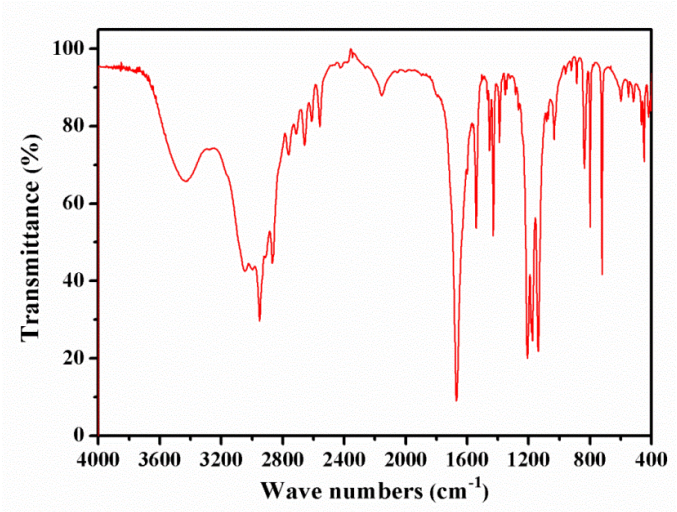

Figure S1. IR spectrum of compound **1**

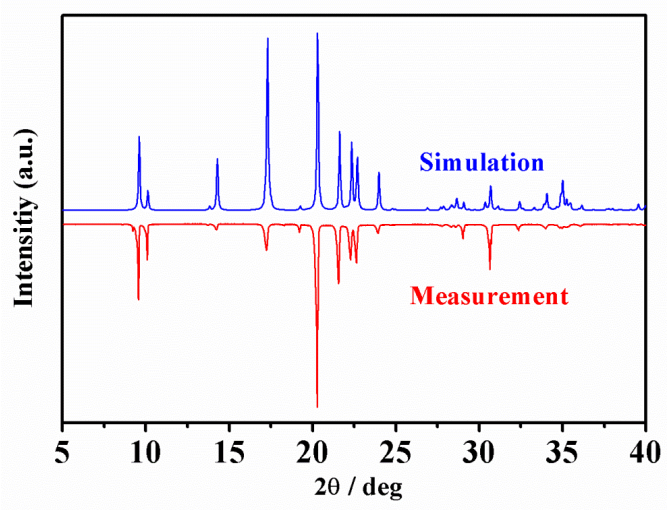

Figure S2. Simulated and experimental XRD powder patterns for compounds **1**.

Table S1. Crystal data and structure refinement of **1** at 100K and 340 K, respectively

Chemical formula	$C_8H_{14}F_3NO_2$	$C_8H_{14}F_3NO_2$
Temperature / K	100(2)	340(2)
Formula weight	213.2	213.2
Crystal system	monoclinic	monoclinic
Space group	*I*2/*a*	*C*2/*m*
a / Å	17.264(3)	18.1351(16)
b / Å	6.5684(2)	6.6817(6)
c / Å	17.7966(19)	9.0685(8)
β / deg	91.40(2)	94.199(7)
Volume / Å^3	2017.5(5)	1095.91(7)
Z	8	4
Dc / g.cm^{-3}	1.404	1.292
R_1 [$I > 2\sigma(I)$]	0.0301	0.1154
ωR_2 [$I > 2\sigma(I)$]	0.0804	0.3411

$\alpha R_1 = \sum ||F_o|-|F_c|| / \sum |F_o|$, $\omega R_2 = [\sum(|F_o|^2-|F_c|^2) / \sum |Fo|^2]^{1/2}$

Single-crystal X-ray structure determination: Data collections were performed on an Agilent technologies Super Nova Micro Focus using Mo-Kα radiation at 100 K and 340 K for **1**. Absorption corrections were applied by using the multi-scan program. The structures were solved by direct methods, and non-hydrogen atoms were refined anisotropically by least-squares on F2 using the SHELXTL-97 program.[1] All the hydrogen atoms were generated geometrically. CCDC 1044765 and 1025090 for **1** contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[1] *SHELXTL 6.10*, Bruker Analytical Instrumentation, Madison, WI, **2000**.

Table S2. Hydrogen-bond geometry (Å, °) in **1**.

100 K	D-H	H···A	D···A	D-H···A
N1-H1A…O1 i	0.89	1.95	2.824	168.6
N1-H1B…O1 ii	0.89	1.93	2.808	170.9
N1-H1C…O2	0.89	1.90	2.786	174.8
340 K				
N1-H1A…O1 i	0.90	1.86	2.749	169.7
N1-H1B…O2 ii	0.90	1.93	2.797	161.5
N1-H1B…O2 iii	0.90	1.93	2.797	161.5
N1-H1A…O2	0.90	2.07	2.905	154.8

Symmetry codes (100 K): (i) x, y-1, z; (ii) –x+1, y-1/2, -z+1/2

Symmetry codes (340 K): (i) x, -y+1, z; (ii) –x+1/2, -y+1/2, -z+1; (iii) –x+1/2, y-1/2, -z+1;

Table S3. The energy density of **1** at different temperature

T **(K)**	***Cp*** **(J· kg^{-1}· K^{-1})**	**Energy Density×10^{6} (J· m^{-3}· K^{-1})**
273	920	1.19
278	949	1.22
283	980	1.27
288	1015	1.31
293	1044	1.35
298	1083	1.40
303	1127	1.46
308	1181	1.53
313	1249	1.61
318	1343	1.74
320	1401	1.81
322	1476	1.91
324	2018	2.61
325	5394	6.97
326	6712	8.67
327	4411	5.70
328	2540	3.28
330	1459	1.89
332	1257	1.62
334	1233	1.59
336	1237	1.60
338	1245	1.61
343	1267	1.64
348	1288	1.66
353	1319	1.70
358	1342	1.73
363	1359	1.76
368	1396	1.80
373	1345	1.85

Table S4. Thermal conductivity for Selected Materials

Compound	Thermal conductivity (W/mK)
Paraffin C18	0.15
Polyglycol E400	0.187
Paraffin C21 – C50	0.21
Naphthalene	0.341
Capric acid	0.16
Lauric acid	0.16
Myristic acid	0.17

The detail of thermal expansion

Solid-solid phase change is always accompanied very little thermal expansion when comparing to solid-liquid, solid-gas phase change. The thermal expansion coefficient can be calculated with the following equation. (L. J. Wang, D. Meng, Appl. Energy, **2010**, 87, 2660.)

$$\alpha = \frac{(V_2 - V_1)}{V_1(T_2 - T_1)} = \frac{\frac{m}{\rho_2} - \frac{m}{\rho_1}}{\frac{m}{\rho_1}(T_2 - T_1)} = \frac{\rho_1 - \rho_2}{\rho_2(T_2 - T_1)}$$

Where α is the volume expansion coefficient of the PCM, V_1 and V_2 are the volume values, ρ_1 and ρ_2 are the density of the PCM at the temperature of T_1 and T_2, respectively. Based on the data, the thermal expansion coefficient of **1** is about 3.6×10^{-4} K^{-1} over the temperature range from 100 K to 340 K, indicating that the compound $[C_6H_{11}NH_3]^+$ $[CF_3COO]^-$ accompanied very little thermal expansion in the phase change process.

The detail measurement of thermal conductivity

Thermal conductivity was calculated on the basis of the following equation:

$$\lambda(T) = \alpha(T) * C_p(T) * \rho(T)$$

Where α is the thermal diffusion coefficient, C_p is specific heat capacity, ρ is the mass density of the compound.

(1) Thermal diffusion coefficient (α) (Figure S4) was measured with powder pellet on a NETZSCH LFA457/2/G via the laser flash method under nitrogen in the temperature range from 313 to 363 K. The powder pellet was prepared under 14 Mpa pressure for 5 min, and diameter of the powder pellet was about 12.7 mm. Each side of the pellet was coated with graphite. The sample holder was graphite one. The laser powder was 1538 V and light transmission was 100%. The data were analysed through direct non-linear regression routines with "Cowan model + Pulse Correction".

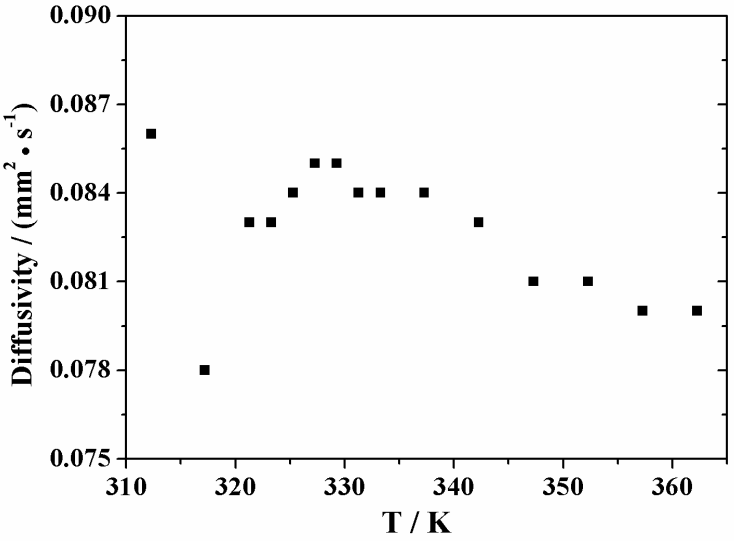

Figure S3. Thermal diffusion coefficient at different temperatures for **1**.

(2) C_p at different temperatures were obtained by heating and cooling the sample (2.516 mg) in an aluminum crucible, and sweeping rate was 10 K· min^{-1} under nitrogen atmosphere in the temperature range of 273-373 K on a NETZSCH DSC 200F3 differential scanning calorimetry.

(3) The values of ρ at different temperatures were taken the one at 340 K, which was obtained through single-crystal data, because thermal expansion of the solid-state sample was very small.