

Supplementary Information for

Colossal Barocaloric Effect in Fatty Acid Methyl Esters

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Specific heat capacity measurement by DSC

Calculation of isobaric entropy change and isothermal entropy change at L-S-T

Under a given external pressure, the isobaric entropy change at L-S-T can be calculated by Eq. (S1) by integrating heat data

$$\Delta S_{LS} = \int_{T_1}^{T_2} \frac{1}{T} \frac{Q(P,T)}{T'} dT \quad (S1)$$

where $Q(P, T)$ is the heat flow after subtracting the baseline, and T' is the scanning rate.

The isothermal entropy change at L-S-T at different pressures is calculated as

$$\Delta S_{P_0 \rightarrow P} = \Delta S_P - \Delta S_{P_0} \quad (S2)$$

Calculation of thermal hysteresis:

The thermal hysteresis (ΔT_{hys}) as an inherent property of first-order phase transition which is at ambient pressure. It is always associated with reversibility of the barocaloric effect. The higher the thermal hysteresis, the lower the reversibility of the barocaloric effect (for refrigeration application, lower thermal hysteresis is important).

It was calculated by subtracting the transition temperature during the cooling process from the ones during the heating process.

$$\Delta T_{hys} = T_H - T_C \quad (S3)$$

T_H represents the peak temperature of the phase transition during heating, while T_C represents the peak temperature of the phase transition during cooling.

Two methods for calculation of refrigeration capacity:

The refrigeration capacity (RC) as the ability of the barocaloric material to carry heat when the temperature difference between the cold and hot ends is large in the ideal refrigeration cycle equipment.

Method 1: According to Wood and Potter's method,¹ the RC value for a reversible refrigeration cycle operating between the hot and cold reservoirs is defined as $RC = \Delta S_{P_0 \rightarrow P}^{max} \cdot \delta T_{FWHM}$ where $\Delta S_{P_0 \rightarrow P}^{max}$ is the maximum entropy change at the hot and cold ends of the cycle (defined equal) and δT_{FWHM} full width at half maximum for $\Delta S_{P_0 \rightarrow P}$.

$$RC = \Delta S_{P_0 \rightarrow P}^{max} \cdot \delta T_{FWHM} \quad (S4)$$

Method 2: The Gschneidner method is to integrate numerically the area below the $\Delta S_M - T$ curve by using the temperatures at half maximum of the peak as the integration limits, which has been widely used in community.²

$$RC = \int_{T_1}^{T_2} \Delta S(T) dT \quad (S5)$$

where T_1 and T_2 are temperatures of the hot and cold sinks at half maximum of the ΔS peak, respectively, and $\Delta S(T)$ is the refrigerants entropy change as a function of temperature.

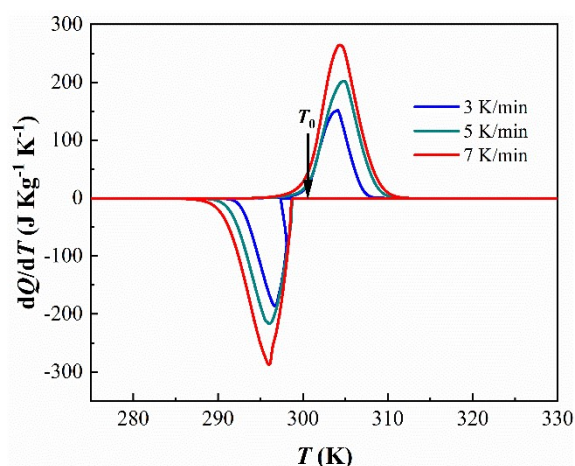


Figure S1. Measurements of dQ/dT after baseline subtraction, on heating ($dQ/dT > 0$) and cooling ($dQ/dT < 0$) across the solid-liquid phase transition, using different temperature ramp rates.

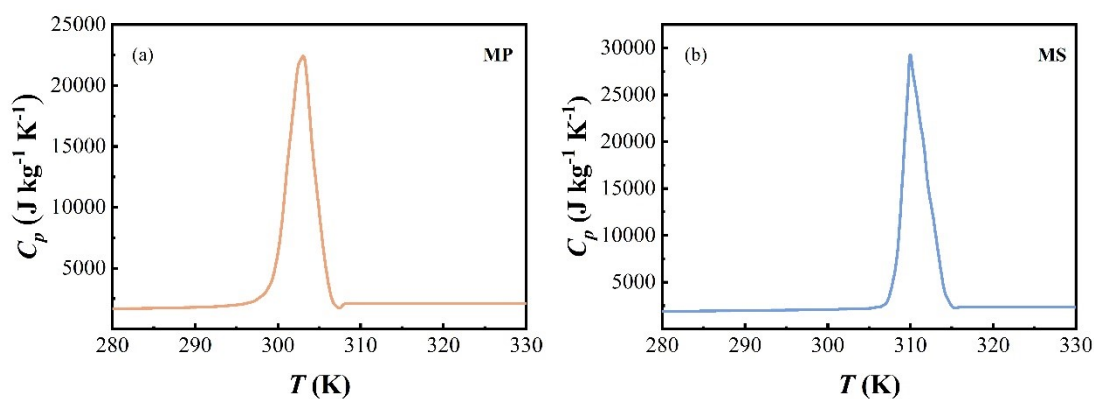


Figure S2. The specific heat capacity data of (a) methyl palmitate (MP) and (b) methyl stearate (MS) measured by DSC at atmospheric pressure with a heating rate of 1 K/min.

Table S1 Raman bands and mode assignments of FAME. Taken from references as indicated.

Band number	Band position(cm^{-1})	Assignments
1	800-920	$\nu(\text{C}_1\text{-C}_2)$, CH_3 , rocking, $\nu(\text{C-O})$: rocking at terminal methyl and increase in acyl chain trans conformation ³
2	1060-1065	$\nu(\text{C-C})_{\text{op}}$ Out-of-phase aliphatic C-C

		stretching all-trans ^{4,5}
3	1080-1110	$\nu(\text{C-C})_g$ Liquid aliphatic C–C stretch in gauche and $\nu(\text{C-C})$ Solid aliphatic C–C stretching in gauche ⁵⁻⁷
4	1100-1135	$\nu(\text{C-C})_{ip}$ In-phase aliphatic C–C stretching all-trans ⁸
5	1295-1305	$\delta(\text{CH}_2)_{tw}$ Methylene twisting deformations ⁹
6	1400-1500	$\delta(\text{CH}_2)_{sc}$ Methylene scissor deformations ⁹
7	1730-1750	$\nu(\text{C=O})$ Carbonyl stretching ⁹
8	2800-2900	$\nu(\text{CH}_2)_s$ and $\nu(\text{CH}_2)_{as}$ ⁷
9	2900-3000	$\nu(\text{CH}_3)_s$ and $\nu(\text{CH}_3)_{as}$ ⁷

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