

Polar Interactions Play an Important Role in the Energetics of the Main Phase Transition of Phosphatidylcholine Membranes

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Supporting Information

Analysis of the differential scanning calorimetric (DSC) thermograms shown in Figs. 2-4. Included are the temperature positions of peaks in the DSC scan (T_m) and the enthalpy change (ΔH) of the total curve, calculated by integration of the heat capacity across the entire transition, as well as the values of T_m and ΔH of sub-curves obtained by deconvolution of the experimental curve using Eq. 7. The experimental curves were deconvolved into either 2 or 3 sub-curves as necessary to provide the best fit of the theoretical curve to the experimental data.

The accuracy of the T_m values are all within ± 0.1 °C.

Table S1: Analysis of DSC thermograms of DMPC containing varying mole percentages of cholesterol (Chol). Experimental data is shown in Fig. 2.

Sample	Total		Sub-curve 1		Sub-curve 2		Sub-curve 3	
	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)
Pure DMPC	23.5	29.8 ± 0.1	23.5	6.3 ± 0.2	23.3	12.9 ± 0.2	23.0	10.1 ± 0.1
Chol 5%	23.3 23.6	29.6 ± 0.1	23.2	1.44 ± 0.05	23.3	11.4 ± 0.1	23.3	16.1 ± 0.1
Chol 7.5%	23.4 23.9	21.1 ± 0.1	23.4	5.17 ± 0.04	23.7	5.8 ± 0.1	24.9	10.1 ± 0.2
Chol 10%	23.3 23.8	22.8 ± 0.1	23.2	5.85 ± 0.03	24.0	2.97 ± 0.05	24.9	13.5 ± 0.1
Chol 12.5%	22.5 23.6	26.9 ± 0.1	23.0	8.5 ± 0.3	26.7	14.3 ± 0.4	26.0	4.5 ± 0.7
Chol 15%	22.1 24.0	27.7 ± 0.1	22.0	1.89 ± 0.03	24.0	5.7 ± 0.1	27.0	19.7 ± 0.1

Table S2: Analysis of DSC thermograms of DMPC containing varying mole percentages of 6-ketocholestanol (6-Keto). Experimental data is shown in Fig. 2.

Sample	Total		Sub-curve 1		Sub-curve 2		Sub-curve 3	
	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)
6-Keto 5%	23.1	23.3 ± 0.1	23.9	9.6 ± 0.1	23.1	8.8 ± 0.1	23.1	4.6 ± 0.1
6-Keto 7.5%	22.7	21.9 ± 0.1	22.6	8.6 ± 0.1	22.7	1.2 ± 0.1	23.7	11.1 ± 0.1
6-Keto 10%	22.1	21.0 ± 0.1	22.8	7.5 ± 0.3	26.7	6.6 ± 0.4	22.0	6.6 ± 0.1
6-Keto 12.5%	21.8 22.2	21.5 ± 0.1	22.6	8.0 ± 0.4	21.7	5.9 ± 0.1	26.3	7.3 ± 0.4
6-Keto 15%	20.9	19.7 ± 0.1	22.7	9.2 ± 0.4	27.6	6.2 ± 0.4	20.7	4.2 ± 0.1

Table S3: Analysis of DSC thermograms of DMPC containing varying mole percentages of 7-ketocholesterol (7-Keto). Experimental data is shown in Fig. 2.

Sample	Total		Sub-curve 1		Sub-curve 2		Sub-curve 3	
	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)
7-Keto 5%	23.5	21.5 ± 0.1	23.5	4.1 ± 0.3	23.5	8.0 ± 0.3	-	-
7-Keto 7.5%	23.3 23.7	19.6 ± 0.1	25.8	6.5 ± 0.2	23.5	7.1 ± 0.2	23.3	5.8 ± 0.1
7-Keto 10%	23.3 23.8	19.2 ± 0.1	23.3	2.6 ± 0.3	23.2	3.2 ± 0.3	24.0	10.0 ± 0.1
7-Keto 12.5%	22.7 23.7	16.4 ± 0.1	23.8	3.8 ± 0.1	22.6	3.27 ± 0.04	26.0	8.9 ± 0.1
7-Keto 15%	21.8 23.2	14.02 ± 0.04	23.5	6.5 ± 0.1	21.5	0.78 ± 0.04	27.6	6.5 ± 0.1

Table S4: Analysis of DSC thermograms of pure DMPC under different solution conditions. Experimental data is shown in Fig. 3.

Sample	Total		Sub-curve 1		Sub-curve 2		Sub-curve 3	
	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)
Buffer + NaCl	23.4	29.6 ± 0.3	23.2	12.9 ± 0.2	23.4	6.3 ± 0.2	23.0	10.1 ± 0.1
Buffer - NaCl	23.9	27.9 ± 0.3	24.0	8.3 ± 0.1	23.9	4.8 ± 0.1	23.0	15.1 ± 0.2
Water	24.1	24.2 ± 0.1	24.1	12.2 ± 0.1	24.3	6.6 ± 0.1	23.4	7.5 ± 0.2

Table S5: Analysis of DSC thermograms of pure DPPC under different solution conditions. Experimental data is shown in Fig. 4.

Sample	Total		Sub-curve 1		Sub-curve 2	
	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)	T _m (°C)	ΔH (kJ/mol)
Buffer + NaCl	41.5	29.2 ± 0.1	41.5	19 ± 4	41.4	8 ± 4
Buffer - NaCl	41.4	28.4 ± 0.1	41.4	21.0 ± 0.2	41.2	5.5 ± 0.2
Water	41.4	34.3 ± 0.1	41.4	20.3 ± 0.4	41.6	13.3 ± 0.5