

Electronic Supplementary Information for “Differential Dependences on $[Ca^{2+}]$ and Temperature of the Monolayer Spontaneous Curvatures of DOPE, DOPA and Cardiolipin: Effects of Modulating the Strength of the Inter-headgroup Repulsion”

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Table S1. The lattice spacing (d), the radius of the cylindrical water core of the H_{II} phase (R_w) and the monolayer spontaneous curvature (C_0) of the DOPE/DOPA and DOPE/cardiolipin mixtures of various molar ratios at varieties of temperatures and $[Ca^{2+}]$ s. The molar percentage indicates the molar ratio of the “guest” species to the total phospholipids in the DOPE/guest mixtures. The values in the parentheses are the C_0 s defined against the *neutral plane*.

$[Ca^{2+}] = 0$ mM

		20 °C					
Lipid		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	d	79.8±0.1	85.0±0.1	86.5	91.7±0.3	94.4±0.2	96.4±0.1
	R_w	21.4±0.2	23.3±0.1	23.8	26.3±0.3	27.3±0.2	28.0±0.1
	C_0	-0.0331±0.0009 (-0.0388±0.0008)	-0.0309±0.0007 (-0.0362±0.0007)	-0.0303±0.0007 (-0.0355±0.0006)	-0.0281±0.0007 (-0.0325±0.0006)	-0.0273±0.0006 (-0.0316±0.0005)	-0.0267±0.0006 (-0.0308±0.0005)
Cardiolipin	d	79.8±0.1	89.5±0.2	94.9±0.2	101.9±0.2	104.8±0.3	110.2±0.2
	R_w	21.4±0.2	25.2±0.3	25.6±0.2	30.2±0.4	30.8	31.5±1.2
	C_0	-0.0331±0.0009 (-0.0388±0.0008)	-0.0291±0.0007 (-0.0338±0.0006)	-0.0278±0.0007 (-0.0333±0.0006)	-0.0251±0.0006 (-0.0289±0.0005)	-0.0244±0.0005 (-0.0284±0.0004)	-0.0235±0.0011 (-0.0279±0.001)

		30 °C					
Lipid		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	d	77.6±0.1	83.2±0.1	83.8	89.7±0.3	92.4±0.2	94.3±0.1
	R_w	20.7±0.3	23.0±0.1	23.4	25.4±0.3	26.6±0.2	27.3±0.1
	C_0	-0.0345±0.0012 (-0.0399±0.0009)	-0.0318±0.0009 (-0.0365±0.0007)	-0.0314±0.0009 (-0.036±0.0006)	-0.0292±0.0009 (-0.0335±0.0007)	-0.0282±0.0008 (-0.0322±0.0006)	-0.0276±0.0007 (-0.0315±0.0005)
Cardiolipin	d	77.6±0.1	87.1±0.2	91.9±0.2	99.1±0.2	102.1±0.3	106.9±0.2
	R_w	20.7±0.3	24.6±0.2	25.2±0.2	28.9±0.3	30.0±0.2	30.5±1.2
	C_0	-0.0345±0.0012 (-0.0399±0.0009)	-0.0301±0.0009 (-0.0344±0.0006)	-0.0288±0.0009 (-0.0338±0.0006)	-0.0262±0.0007 (-0.0301±0.0005)	-0.0253±0.0007 (-0.0291±0.0005)	-0.0245±0.0013 (-0.0287±0.0011)

		40 °C					
Lipid		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	d	75.3±0.1	81.3±0.1	81.2	87.0±0.3	89.9±0.2	91.6±0.1
	R_w	19.9±0.4	22.3±0.2	22.0	24.3±0.3	25.7±0.2	26.3±0.1
	C_0	-0.0365±0.0014 (-0.0412±0.0011)	-0.0334±0.0010 (-0.0375±0.0007)	-0.0336±0.0009 (-0.0379±0.0007)	-0.0309±0.0009 (-0.0348±0.0007)	-0.0297±0.0008 (-0.0333±0.0006)	-0.0291±0.0007 (-0.0326±0.0005)
Cardiolipin	d	75.3±0.1	84.4±0.2	89.1±0.2	96.2±0.2	99.3±0.3	103.4±0.2
	R_w	19.9±0.4	23.5±0.1	24.5±0.2	28.1	28.9±0.2	29.4±1.1
	C_0	-0.0365±0.0014 (-0.0412±0.0011)	-0.0320±0.0009 (-0.0359±0.0007)	-0.0304±0.0009 (-0.0347±0.0006)	-0.0275±0.0007 (-0.0308±0.0005)	-0.0267±0.0007 (-0.0301±0.0005)	-0.0259±0.0013 (-0.0296±0.0011)

$[Ca^{2+}] = 10$ mM

		20 °C					
Lipid		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	d	77.9±0.1	83.4±0.3	-	-	-	-
	R_w	20.7±0.1	22.0±0.3	-	-	-	-
	C_0	-0.0340±0.0009 (-0.0399±0.0008)	-0.0318±0.0009 (-0.0378±0.0008)	-	-	-	-
Cardiolipin	d	77.9±0.1	-	90.6±0.3	-	97.4±0.3	101.9±0.2
	R_w	20.7±0.1	-	25.6±0.3	-	28.5±0.3	30.1±0.2
	C_0	-0.0340±0.0009 (-0.0399±0.0008)	-	-0.0287±0.0007 (-0.0333±0.0006)	-	-0.0263±0.0007 (-0.0304±0.0006)	-0.0251±0.0006 (-0.0290±0.0005)

		30 °C						
Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		75.7±0.1	82.2±0.3	-	-	-	-
	<i>R_w</i>		20.0±0.1	21.7±0.3	-	-	-	-
	<i>C₀</i>		-0.0355±0.0011 (-0.0410±0.0009)	-0.0326±0.0011 (-0.0383±0.0008)	-	-	-	-
Cardiolipin	<i>d</i>		75.7±0.1	-	88.2±0.3	-	95.1±0.3	98.8±0.2
	<i>R_w</i>		20.0±0.1	-	24.7±0.3	-	27.5±0.3	28.9±0.2
	<i>C₀</i>		-0.0355±0.0011 (-0.0410±0.0009)	-	-0.0298±0.0009 (-0.0344±0.0007)	-	-0.0274±0.0008 (-0.0314±0.0006)	-0.0262±0.0007 (-0.03±0.0005)

		40 °C						
Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		73.4±0.1	80.3±0.3	-	-	-	-
	<i>R_w</i>		19.2±0.1	21.2±0.3	-	-	-	-
	<i>C₀</i>		-0.0376±0.0011 (-0.0424±0.0009)	-0.0343±0.0011 (-0.0391±0.0009)	-	-	-	-
Cardiolipin	<i>d</i>		73.4±0.1	-	85.6±0.3	-	92.5±0.3	95.8±0.2
	<i>R_w</i>		19.2±0.1	-	23.7±0.3	-	26.5±0.3	27.9±0.2
	<i>C₀</i>		-0.0376±0.0011 (-0.0424±0.0009)	-	-0.0316±0.0010 (-0.0356±0.0007)	-	-0.0288±0.0008 (-0.0323±0.0006)	-0.0276±0.0007 (-0.0309±0.0005)

[Ca²⁺] = 20 mM

		20 °C						
Lipid		Fraction	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		77.3	-	-	-	-	-
	<i>R_w</i>		20.8	-	-	-	-	-
	<i>C₀</i>		-0.0342±0.0008 (-0.0397±0.0008)	-	-	-	-	-
Cardiolipin	<i>d</i>		77.3	-	91.7±0.1	94.8±0.1	98.6±0.3	100.6±0.1
	<i>R_w</i>		20.8	-	26.2±0.1	27.5±0.1	29.0±0.3	29.8±0.1
	<i>C₀</i>		-0.0342±0.0008 (-0.0397±0.0008)	-	-0.0282±0.0006 (-0.0327±0.0006)	-0.0271±0.0006 (-0.0313±0.0005)	-0.0260±0.0006 (-0.03±0.0005)	-0.0254±0.0005 (-0.0292±0.0004)

		30 °C						
Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		75.1	-	-	-	-	-
	<i>R_w</i>		20.1	-	-	-	-	-
	<i>C₀</i>		-0.0356±0.0010 (-0.0409±0.0008)	-	-	-	-	-
Cardiolipin	<i>d</i>		75.1±	-	90.0±0.1	93.1±0.1	96.7±0.3	98.7±0.1
	<i>R_w</i>		20.1	-	25.7±0.1	26.8±0.1	28.1±0.3	29.2±0.1
	<i>C₀</i>		-0.0356±0.0010 (-0.0409±0.0008)	-	-0.0290±0.0008 (-0.0333±0.0006)	-0.0279±0.0007 (-0.032±0.0005)	-0.0268±0.0007 (-0.0307±0.0005)	-0.0261±0.0007 (-0.0298±0.0005)

		40 °C						
Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		73.0	-	-	-	-	-
	<i>R_w</i>		19.3	-	-	-	-	-
	<i>C₀</i>		-0.0377±0.0011 (-0.0422±0.0009)	-	-	-	-	-
Cardiolipin	<i>d</i>		73.0	-	87.6±0.1	90.9±0.1	94.5±0.3	96.5±0.1
	<i>R_w</i>		19.3	-	24.7±0.1	26.0±0.1	27.4±0.3	28.4±0.1
	<i>C₀</i>		-0.0377±0.0011 (-0.0422±0.0009)	-	-0.0306±0.0008 (-0.0344±0.0006)	-0.0293±0.0008 (-0.0328±0.0006)	-0.0281±0.0008 (-0.0314±0.0006)	-0.0273±0.0007 (-0.0305±0.0005)

[Ca²⁺] = 50 mM

		20 °C						
Lipid		Fraction	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		78.0	82.4±1.0	84.2±0.2	86.0±0.3	84.7	84.7±0.4
	<i>R_w</i>		20.2	22.3±1.0	22.7±0.6	23.1±0.7	22.5	23.0±0.4
	<i>C₀</i>		-0.0343±0.0009 (-0.0406±0.0008)	-0.0319±0.0010 (-0.0374±0.0009)	-0.0313±0.0012 (-0.0369±0.0011)	-0.0307±0.0013 (-0.0364±0.0011)	-0.0313±0.0008 (-0.0371±0.0007)	-0.0311±0.0010 (-0.0365±0.0009)

Cardiolipin	<i>d</i>	78.0	-	87.8±0.2	90.0±0.1	92.8	95.7±0.1
	<i>R_w</i>	20.2	-	24.9±0.2	25.6±0.1	26.8	27.9±0.1
	<i>C₀</i>	-0.0343±0.0009 (-0.0406±0.0008)	-	-0.0295±0.0007 (-0.0342±0.0006)	-0.0288±0.0007 (-0.0334±0.0006)	-0.0278±0.0006 (-0.032±0.0005)	-0.0268±0.0006 (-0.0309±0.0005)

30 °C

Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		76.3	81.2±1.0	82.6±0.2	84.4±0.3	83.4	83.1±0.4
	<i>R_w</i>		19.7	21.9±1.0	22.2±0.5	22.8±0.6	22.1	22.8±0.4
	<i>C₀</i>		-0.0355±0.0011 (-0.0415±0.0009)	-0.0329±0.0011 (-0.0381±0.0008)	-0.0323±0.0013 (-0.0376±0.001)	-0.0316±0.0013 (-0.0368±0.001)	-0.0322±0.0009 (-0.0377±0.0007)	-0.0319±0.0011 (-0.0368±0.0009)
Cardiolipin	<i>d</i>		76.3	-	86.2±0.2	88.6±0.1	91.1	93.9±0.1
	<i>R_w</i>		19.7	-	24.2±0.2	25.3±0.1	26.1	27.2±0.1
	<i>C₀</i>		-0.0355±0.0011 (-0.0415±0.0009)	-	-0.0305±0.0009 (-0.035±0.0006)	-0.0295±0.0008 (-0.0337±0.0006)	-0.0286±0.0008 (-0.0328±0.0005)	-0.0277±0.0007 (-0.0317±0.0005)

40 °C

Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		74.3	79.4±1.0	81.0±0.2	82.9±0.3	82.0	81.5±0.4
	<i>R_w</i>		19.0	21.3±1.0	21.7±0.6	22.3±0.6	21.7	22.5±0.4
	<i>C₀</i>		-0.0374±0.0011 (-0.0427±0.0009)	-0.0345±0.0011 (-0.039±0.0008)	-0.0338±0.0015 (-0.0383±0.0012)	-0.0329±0.0014 (-0.0374±0.0011)	-0.0336±0.0010 (-0.0384±0.0007)	-0.0332±0.0011 (-0.0372±0.0009)
Cardiolipin	<i>d</i>		74.3	-	84.4±0.2	86.9±0.1	89.2	91.6±0.1
	<i>R_w</i>		19.0	-	23.6±0.2	24.5±0.1	25.4	26.3±0.1
	<i>C₀</i>		-0.0374±0.0011 (-0.0427±0.0009)	-	-0.0319±0.0009 (-0.0358±0.0007)	-0.0309±0.0008 (-0.0346±0.0006)	-0.0300±0.0008 (-0.0336±0.0006)	-0.0291±0.0007 (-0.0325±0.0005)

[Ca²⁺] = 70 mM

Lipid		Fraction	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		77.8±0.1	-	81.4±0.2	82.6±0.3	82.2±0.2	84.6±0.1
	<i>R_w</i>		20.2±0.1	-	21.5±0.2	21.7±0.3	21.8±0.2	22.5±0.1
	<i>C₀</i>		-0.0343±0.0009 (-0.0406±0.0008)	-	-0.0326±0.0009 (-0.0386±0.0008)	-0.0322±0.001 (-0.0383±0.0009)	-0.0323±0.0009 (-0.0382±0.0008)	-0.0313±0.0008 (-0.0372±0.0007)
Cardiolipin	<i>d</i>		77.8±0.1	-	-	-	-	-
	<i>R_w</i>		20.2±0.1	-	-	-	-	-
	<i>C₀</i>		-0.0343±0.0009 (-0.0406±0.0008)	-	-	-	-	-

30 °C

Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		76.3±0.1	-	79.9±0.2	81.1±0.3	80.7±0.2	83.3±0.1
	<i>R_w</i>		19.8±0.1	-	21.1±0.2	21.4±0.3	21.7±0.2	22.0±0.1
	<i>C₀</i>		-0.0354±0.0011 (-0.0414±0.0009)	-	-0.0336±0.0011 (-0.0392±0.0008)	-0.0331±0.0012 (-0.0388±0.0009)	-0.0331±0.0010 (-0.0384±0.0008)	-0.0322±0.0010 (-0.0378±0.0007)
Cardiolipin	<i>d</i>		76.3±0.1	-	-	-	-	-
	<i>R_w</i>		19.8±0.1	-	-	-	-	-
	<i>C₀</i>		-0.0354±0.0011 (-0.0414±0.0009)	-	-	-	-	-

40 °C

Lipid		[Ca ²⁺]	0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
DOPA	<i>d</i>		74.5±0.1	-	78.4±0.2	79.6±0.3	79.3±0.2	81.8±0.1
	<i>R_w</i>		19.1±0.1	-	20.6±0.2	21.0±0.3	22.3±0.2	21.6±0.1
	<i>C₀</i>		-0.0373±0.0011 (-0.0426±0.0009)	-	-0.0352±0.0011 (-0.0401±0.0009)	-0.0346±0.0012 (-0.0394±0.0009)	-0.0339±0.0010 (-0.0375±0.0008)	-0.0336±0.0010 (-0.0385±0.0008)
Cardiolipin	<i>d</i>		74.5±0.1	-	-	-	-	-
	<i>R_w</i>		19.1±0.1	-	-	-	-	-
	<i>C₀</i>		-0.0373±0.0011 (-0.0426±0.0009)	-	-	-	-	-

[Ca²⁺] = 100 mM

		20 °C					
Fraction		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
Lipid	<i>d</i>	75.5±0.1	-	-	77.6±0.1	-	78.6±0.3
	<i>R_w</i>	20.7±0.1	-	-	20.7±0.1	-	21.0±0.3
	<i>C₀</i>	-0.0347±0.0009 (-0.0398±0.0008)	-	-	-0.0341±0.0008 (-0.0398±0.0008)	-	-0.0336±0.0008 (-0.0393±0.0008)
Cardiolipin	<i>d</i>	75.5±0.1	80.4±0.8	83.8±0.3	86.0±0.1	88.1±0.2	90.1±0.2
	<i>R_w</i>	20.7±0.1	21.6±0.8	22.9±0.3	23.7±0.1	24.2±0.2	25.5±0.2
	<i>C₀</i>	-0.0347±0.0009 (-0.0398±0.0008)	-0.0328±0.0016 (-0.0384±0.0014)	-0.0314±0.0009 (-0.0367±0.0008)	-0.0305±0.0007 (-0.0356±0.0006)	-0.0297±0.0008 (-0.0349±0.0007)	-0.0288±0.0007 (-0.0335±0.0006)
		30 °C					
[Ca ²⁺]		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
Lipid	<i>d</i>	74.3±0.1	-	-	77.1±0.1	-	78.8±0.3
	<i>R_w</i>	20.5±0.1	-	-	20.5±0.1	-	21.0±0.3
	<i>C₀</i>	-0.0356±0.0010 (-0.0402±0.0008)	-	-	-0.0348±0.0010 (-0.0402±0.0008)	-	-0.0340±0.0010 (-0.0394±0.0008)
Cardiolipin	<i>d</i>	74.3±0.1	78.9±0.8	82.1±0.3	84.4±0.1	86.2±0.2	88.3±0.2
	<i>R_w</i>	20.5±0.1	21.2±0.8	22.3±0.3	23.1±0.1	23.6±0.2	24.9±0.2
	<i>C₀</i>	-0.0356±0.0010 (-0.0402±0.0008)	-0.0339±0.0017 (-0.0391±0.0014)	-0.0324±0.0010 (-0.0374±0.0008)	-0.0315±0.0009 (-0.0364±0.0007)	-0.0308±0.0009 (-0.0358±0.0007)	-0.0297±0.0009 (-0.0341±0.0006)
		40 °C					
[Ca ²⁺]		0 mol%	10 mol%	15 mol%	20 mol%	25 mol%	30 mol%
Lipid	<i>d</i>	-	-	-	76.2±0.1	80.4±0.4	78.5±0.3
	<i>R_w</i>	-	-	-	20.0±0.1	22.0±0.4	20.9±0.3
	<i>C₀</i>	-	-	-	-0.0362±0.0011 (-0.041±0.0009)	-0.0337±0.0012 (-0.0378±0.0009)	-0.0350±0.0010 (-0.0395±0.0008)
Cardiolipin	<i>d</i>	-	77.2±0.8	80.3±0.3	82.8±0.1	84.2±0.2	86.5±0.2
	<i>R_w</i>	-	20.6±0.8	21.7±0.3	22.4±0.1	22.8±0.2	24.3±0.2
	<i>C₀</i>	-	-0.0355±0.0018 (-0.04±0.0015)	-0.0340±0.0011 (-0.0383±0.0009)	-0.0329±0.0009 (-0.0373±0.0007)	-0.0324±0.0010 (-0.0367±0.0007)	-0.0311±0.0009 (-0.0349±0.0007)

Uncertainty estimation associated with a linear fitting

This section describes the statistical method employed in the present study to estimate the uncertainty related to the *C₀*s of DOPA and cardiolipin, which were determined through linear extrapolations. The *C₀*s along with their associated uncertainty is summarized in Table 1 of the main text.

At $x = x$, the uncertainty related to the value, y , determined by extrapolating or interpolating the linear correlation, $y = ax + b$, for n data points, (x_i, y_i) , is,

$$y_uncertainty = t_{\alpha/2, n-2} \cdot S \cdot \sqrt{\frac{1}{n} + \frac{n(x - \bar{x})^2}{n \sum x_i^2 - (\sum x_i)^2}}$$

and

$$S = \sqrt{\frac{\sum (y_i - ax_i - b)^2}{n - 2}}$$

where $(1 - \alpha) \times 100\%$ is the confidence level, \bar{x} is the average of x_i and $t_{\alpha/2, n-2}$ is the critical value for the t -distribution. In the present study, the confidence level of 95% was employed and the number of data points for a linear fitting was mostly 5 or 6. Therefore, the value of $t_{\alpha/2, n-2}$ was mostly 3.182 or 2.776. For the present study, (x_i, y_i) = (molar ratio of the guest species, collective *C₀* of the mixture) and are presented above.