Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

New polymorphic phase of arachidic-acid crystal: structural, intermolecular interactions, low-temperature stability and Raman spectroscopy combined with DFT calculations

Luanny M. B. Cardoso,[a] João G. de Oliveira Neto,[b] Gilberto D. Saraiva,[c] Fábio F. Leite,[d] Alejandro. P. Ayala,[e] Adenilson O. dos Santos,[a] and Francisco F. de Sousa[a,b,*]

[a]Institute of Exact and Natural Sciences, Federal University of Para - UFPA, Belém, Pará, CEP 66075-110, Brazil

[b]Center for Social Sciences, Health, and Technology, Federal University of Maranhao - UFMA, Imperatriz, Maranhão, CEP 65900-410, Brazil

[c]Physics Course, State University of Ceara-UECE, Campus FECLESC, Quixadá, Ceará, CEP 63900-000, Brazil

[d]Department of Exact and Technological Sciences, Federal University of Amapá - UNIFAP, Macapá, Amapá, CEP 68903-419, Brazil

[e]Department of Physics, Federal University of Ceara - UFC, Fortaleza, CE 65455-900, Brazil

*Corresponding author: ffs@ufpa.br (F. F. Sousa)

Table S1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for the AA crystal at 100 K and 300 K. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

	100 K				300 K			
Atom	***x***	***y***	***z***	**U(eq)**	***x***	***y***	***z***	**U(eq)**
O1	4675.2(2)	4210.9(17)	10386(2)	18.9(3)	4677.6(4)	4230(3)	10388(4)	60.9(7)
O2	4914.2(2)	6341.6(17)	12612(2)	19.7(3)	4910.7(4)	6306(3)	12556(4)	64.8(8)
C1	4696.5(3)	5263(2)	12134(3)	16.5(4)	4695.9(6)	5252(5)	12103(6)	50.3(9)
C4	4037.3(3)	5398(2)	11265(3)	15.8(4)	4040.5(6)	5387(4)	11195(6)	46.5(8)
C6	3573.5(3)	5418(2)	8836(3)	16.0(4)	3576.7(6)	5400(4)	8757(6)	45.4(8)
C2	4482.4(3)	5462(2)	13989(3)	17.5(4)	3287.8(6)	4607(4)	8443(6)	47.2(8)
C8	3107.0(3)	5424(2)	6463(3)	15.9(4)	3751.1(6)	4577(4)	10829(6)	46.6(8)
C5	3748.5(3)	4558(2)	10930(3)	15.9(4)	2822.8(6)	4606(4)	6086(6)	48.6(8)
C7	3283.6(3)	4587(2)	8561(3)	16.3(4)	3111.0(6)	5403(4)	6367(6)	46.3(8)
C3	4208.0(3)	4492(2)	13361(3)	16.7(4)	4210.5(6)	4507(5)	13261(6)	50.0(8)
C10	2639.4(3)	5417(2)	4113(3)	15.7(4)	2356.3(6)	4608(4)	3731(6)	50.6(8)
C12	2171.8(3)	5418(2)	1774(3)	16.2(4)	2644.3(6)	5395(4)	4007(6)	48.8(8)
C9	2817.4(3)	4589(2)	6208(3)	16.1(4)	2177.3(6)	5394(5)	1661(6)	50.6(8)
C13	1881.1(3)	4589(2)	1538(3)	16.0(4)	1888.2(6)	4618(5)	1392(6)	53.3(9)
C11	2349.5(3)	4588(2)	3866(3)	16.4(4)	1708.2(6)	5387(5)	-663(6)	52.8(9)
C15	1412.6(3)	4590(2)	-788(3)	16.5(4)	4485.2(6)	5426(5)	13905(6)	55.1(9)
C14	1703.7(3)	5421(2)	-553(3)	16.4(4)	1419.9(6)	4616(5)	-921(6)	55.8(9)
C17	943.1(4)	4589(2)	-3081(3)	17.8(4)	950.9(7)	4612(5)	-3195(6)	60.7(10)
C16	1233.6(3)	5423(2)	-2868(3)	17.1(4)	1238.4(6)	5384(5)	-2959(6)	56.3(9)
C18	762.1(4)	5411(2)	-5150(3)	19.3(4)	764.8(7)	5374(5)	-5223(7)	63.6(10)
C19	473.4(4)	4555(3)	-5367(3)	22.2(4)	479.5(7)	4584(6)	-5444(7)	78.8(13)
C20	290.2(4)	5389(3)	-7418(4)	28.2(5)	293.0(9)	5353(7)	-7452(9)	97.7(15)

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for the AA crystal at 100 K. The Anisotropic displacement factor exponent is $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	20.3(6)	18.6(6)	17.8(7)	-5.1(5)	0.4(5)	0.2(5)
O2	18.7(6)	22.4(7)	18.2(7)	-4.2(5)	2.7(5)	-4.0(5)
C1	17.8(9)	15.4(8)	16.0(9)	2.8(6)	-2.4(6)	1.3(6)
C4	13.9(8)	15.8(8)	17.6(9)	0.3(6)	-0.5(6)	0.3(6)
C6	14.2(8)	16.8(9)	16.9(9)	0.8(6)	-1.3(6)	-0.8(6)
C2	15.8(8)	22.9(9)	13.5(8)	-1.3(7)	-1.6(6)	-0.3(6)
C8	15.4(8)	17.0(9)	15.1(9)	0.8(6)	-1.6(6)	-0.5(6)
C5	15.2(8)	17.3(9)	15.0(8)	1.0(6)	-0.1(6)	0.1(6)
C7	14.5(8)	17.9(9)	16.3(9)	0.6(6)	-0.4(6)	-0.3(6)
C3	15.5(8)	20.6(9)	14.0(9)	1.9(6)	0.7(6)	0.2(6)
C10	15.4(8)	16.7(9)	14.7(8)	1.2(6)	-1.5(6)	0.4(6)
C12	16.8(8)	17.7(9)	14.0(9)	0.9(6)	-1.0(6)	-0.3(6)
C9	14.6(8)	17.5(9)	16.0(9)	0.2(6)	-2.0(6)	0.6(6)
C13	17.2(8)	16.9(9)	13.7(9)	1.0(6)	-1.9(6)	-0.2(6)
C11	16.2(8)	17.4(9)	15.5(9)	0.5(6)	-1.6(6)	0.1(6)
C15	17.7(8)	16.5(9)	15.0(9)	1.0(6)	-1.7(6)	-0.5(6)
C14	16.8(8)	17.9(9)	14.3(9)	1.5(6)	-1.6(6)	-0.6(6)
C17	19.7(9)	17.6(9)	15.8(9)	1.3(7)	-1.8(7)	-0.5(6)
C16	17.3(8)	18.8(9)	15.1(9)	2.3(6)	-1.1(6)	0.0(6)
C18	19.1(9)	21.4(9)	16.9(9)	1.4(7)	-1.9(7)	0.6(7)
C19	21.3(9)	25.6(10)	19.3(10)	1.9(7)	-2.1(7)	-0.3(7)
C20	22.4(10)	37.1(12)	24.5(11)	0.7(8)	-5.6(8)	1.3(8)

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for the AA crystal at 300 K. The Anisotropic displacement factor exponent is $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	50.5(14)	73.9(17)	58.9(16)	-17.1(13)	8.7(11)	-4.6(11)
O1	54.6(14)	78.4(18)	62.3(17)	-15.7(13)	12.2(11)	-13.8(12)
C1	41.8(18)	60(2)	49(2)	5.2(18)	-3.5(14)	2.9(15)
C4	39.3(16)	50(2)	50.1(19)	-0.6(15)	1.7(14)	-2.0(13)
C6	41.3(16)	50(2)	44.8(18)	1.7(15)	0.3(13)	0.7(13)
C7	41.1(16)	53(2)	47.0(19)	0.1(15)	0.6(13)	-0.1(14)
C5	41.8(17)	49(2)	48.5(19)	2.6(15)	3.2(14)	-0.8(13)
C9	43.2(17)	55(2)	47.2(19)	0.1(15)	-3.2(14)	1.9(14)
C8	41.6(17)	53(2)	43.6(18)	1.4(15)	-1.3(13)	0.2(14)
C3	42.0(17)	61(2)	47.1(19)	3.8(16)	6.3(14)	-0.6(14)
C11	45.2(18)	59(2)	46.4(19)	-2.0(16)	-3.8(14)	0.0(15)
C10	45.3(17)	54(2)	47.1(19)	3.7(15)	-1.6(14)	-1.0(14)
C12	45.7(18)	60(2)	45.1(19)	4.9(16)	-1.9(14)	-1.6(15)
C13	49.2(19)	65(2)	45.2(19)	1.2(16)	-3.8(15)	-0.4(15)
C14	47.6(18)	68(2)	42.7(19)	5.0(16)	-2.5(14)	1.1(15)
C2	44.1(18)	74(3)	47(2)	-2.5(17)	1.5(15)	-0.8(15)
C15	48.8(19)	73(3)	45(2)	2.5(17)	-3.7(15)	0.1(16)
C17	52(2)	77(3)	52(2)	1.3(18)	-4.3(16)	2.2(17)
C16	47.3(19)	73(3)	47(2)	3.8(17)	-3.1(15)	1.0(16)
C18	52(2)	82(3)	56(2)	0.9(19)	-4.7(16)	1.7(18)
C19	56(2)	110(4)	69(3)	4(2)	-6.5(19)	-3(2)
C20	66(3)	142(4)	83(3)	6(3)	-16(2)	4(3)

Table S4. Bond lengths for AA crystal at 100 K and 300 K.

		100 K	300 K			100 K	300 K
Atom	Atom	Length (Å)		Atom	Atom	Length (Å)	
O1	C1	1.225(2)	1.314(4)	C10	C11	1.525(2)	1.513(4)
O2	C1	1.323(2)	1.221(4)	C12	C13	1.528(2)	1.514(4)
C1	C2	1.500(2)	1.481(5)	C12	C11	1.527(2)	1.522(4)
C4	C5	1.525(2)	1.528(4)	C13	C14	1.527(2)	1.514(4)
C4	C3	1.534(2)	1.527(4)	C15	C14	1.530(2)	1.509(4)
C6	C5	1.530(2)	1.522(4)	C15	C16	1.527(2)	1.511(4)
C6	C7	1.526(2)	1.519(4)	C17	C16	1.528(2)	1.505(4)
C2	C3	1.524(2)	1.520(4)	C17	C18	1.525(2)	1.517(5)
C8	C7	1.529(2)	1.522(4)	C18	C19	1.526(2)	1.500(5)
C8	C9	1.525(2)	1.516(4)	C19	C20	1.527(2)	1.513(5)
C10	C9	1.529(2)	1.525(4)				

Table S5. Bond angles for AA crystal at 100 and 300 K.

			100 K	300 K				100 K	300 K
Atoms			Angle (°)		Atoms			Angle (°)	
O1	C1	O2	123.47(16)	122.7(3)	C11	C12	C13	113.42(14)	114.5(3)
O1	C1	C2	124.25(15)	112.8(3)	C8	C9	C10	113.64(14)	114.1(3)
O2	C1	C2	112.27(14)	124.6(3)	C14	C13	C12	113.36(14)	115.0(3)
C5	C4	C3	112.53(14)	112.7(3)	C10	C11	C12	113.55(14)	114.4(3)
C7	C6	C5	113.11(14)	113.7(3)	C16	C15	C14	113.55(14)	115.2(3)
C1	C2	C3	115.18(14)	115.4(3)	C13	C14	C15	113.30(14)	114.9(3)
C9	C8	C7	113.30(14)	113.8(3)	C18	C17	C16	113.66(14)	115.6(3)
C4	C5	C6	113.88(14)	114.2(3)	C15	C16	C17	113.13(14)	114.8(3)
C6	C7	C8	113.69(14)	114.5(3)	C17	C18	C19	113.32(15)	115.0(3)
C2	C3	C4	114.34(14)	114.6(3)	C18	C19	C20	113.51(15)	115.0(4)
C11	C10	C9	113.60(14)	114.2(3)					

Table S6. Hydrogen bonds for the AA crystal at 100 and 300 K.

Temperature (K)	D	H	A	d(D-H) (Å)	d(H-A) (Å)	d(D-A) (Å)	D-H-A (°)
100	O1	H1	O2[1]	0.84	1.84	2.679(4)	173.9
300	O1	H1	O2[1]	0.82	1.88	2.689(3)	171.2

[1]*1-x, 1-y, 2-z*

Table S7. Torsion angles for the AA crystal at 100 K.

A	B	C	D	Angle (˚)	A	B	C	D	Angle (˚)
O1	C1	C2	C3	-9.6(2)	C9	C10	C11	C12	179.94(14)
O2	C1	C2	C3	171.11(14)	C13	C12	C11	C10	-179.81(13)
C1	C2	C3	C4	-69.70(19)	C11	C10	C9	C8	-179.72(13)
C5	C4	C3	C2	-171.96(14)	C11	C12	C13	C14	179.95(14)
C5	C6	C7	C8	-179.60(14)	C14	C15	C16	C17	-179.78(14)
C7	C6	C5	C4	-178.88(13)	C17	C18	C19	C20	179.33(15)
C7	C8	C9	C10	-179.95(14)	C16	C15	C14	C13	179.72(14)
C3	C4	C5	C6	-179.42(13)	C16	C17	C18	C19	179.36(14)
C12	C13	C14	C15	-179.99(13)	C18	C17	C16	C15	179.93(14)
C9	C8	C7	C6	-179.82(14)					

Table S8. Torsion angles for the AA crystal at 300 K.

A	B	C	D	Angle (˚)	A	B	C	D	Angle (˚)
O1	C1	C2	C3	169.5(3)	C9	C10	C11	C12	179.9(3)
O2	C1	C2	C3	-11.4(5)	C13	C12	C11	C10	-179.6(3)
C1	C2	C3	C4	-69.1(4)	C11	C10	C9	C8	-179.7(3)
C5	C4	C3	C2	-172.4(4)	C11	C12	C13	C14	-179.9(3)
C5	C6	C7	C8	-179.5(5)	C14	C15	C16	C17	-179.7(3)
C7	C6	C5	C4	-178.9(2)	C17	C18	C19	C20	179.5(3)
C7	C8	C9	C10	-180.0(3)	C16	C15	C14	C13	179.7(3)
C3	C4	C5	C6	-179.1(3)	C16	C17	C18	C19	179.6(3)
C12	C13	C14	C15	-179.8(3)	C18	C17	C16	C15	179.6(3)
C9	C8	C7	C6	-179.7(3)					

Table S9. Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) for the AA crystal at 100 K.

Atom	*x*	*y*	*z*	U(eq)
H2	5034.63	6125.61	11604.92	30
H4A	4021.04	6756.02	11577.42	19
H4B	4135.38	5238.02	9748.79	19
H6A	3558.55	6782.45	9103.7	19
H6B	3668.59	5224.86	7310.27	19
H2A	4446.56	6810.41	14231.72	21
H2B	4559.06	4953.36	15546.61	21
H8A	3091.64	6790.19	6711.59	19
H8B	3201.35	5219.28	4936.23	19
H5A	3650.91	4727.75	12447.82	19
H5B	3765.8	3197.49	10643.72	19
H7A	3188.64	4786.98	10085.87	20
H7B	3299.11	3220.8	8309	20
H3A	4096.68	4487.01	14816.52	20
H3B	4245.22	3174.14	12934.96	20
H10A	2624.5	6784.37	4352.88	19
H10B	2733.03	5206.23	2583.22	19

H12A	2264.95	5204.38	243.21	19
H12B	2157.3	6785.6	2013.47	19
H9A	2723.29	4793.62	7736.27	19
H9B	2833.03	3221.96	5963.43	19
H13A	1895.53	3220.78	1296.45	19
H13B	1787.94	4800.87	3068.89	19
H11A	2255.88	4797	5396.28	20
H11B	2364.34	3220.28	3624	20
H15A	1427.25	3222.44	-1035.26	20
H15B	1320.05	4795.97	747.88	20
H14A	1796.76	5208.34	-2084.65	20
H14B	1689.19	6788.65	-312.21	20
H17A	958.05	3221.26	-3322.02	21
H17B	851.92	4798.25	-1539.04	21
H16A	1325.38	5211.3	-4406.56	21
H16B	1219.12	6790.51	-2625.46	21
H18A	854.01	5213.74	-6690.72	23
H18B	745.08	6776.2	-4899.45	23
H19A	382.47	4738.34	-3818.28	27
H19B	490.5	3191.62	-5635.46	27
H20A	377.12	5196.11	-8963.22	42
H20B	266.86	6732.31	-7138.51	42
H20C	109.19	4775.35	-7469.3	42

Table S10. Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) for the AA crystal at 300 K.

Atom	***x***	***y***	***Z***	**U(eq)**
H1	5034.17	6027.44	11683.89	97
H4A	4136.78	5242.35	9734.56	56
H4B	4024.63	6670.72	11505.61	56
H6A	3562.11	6691.25	9016.04	54
H6B	3670.46	5218.95	7291.05	54
H7A	3194.19	4795.91	9908.73	57
H7B	3303.01	3313.94	8202.98	57
H5A	3768.21	3288.66	10552.62	56
H5B	3655.2	4735.79	12287.69	56
H9A	2730.55	4802.12	7556.29	58
H9B	2838.07	3311.75	5855.22	58
H8A	3095.97	6697.34	6600.7	56
H8B	3203.47	5207.51	4897.54	56
H3A	4101.74	4503.44	14662.32	60
H3B	4245.64	3258.98	12846.05	60
H11A	2264.66	4807.07	5203.47	61
H11B	2370.96	3313.15	3502.46	61
H10A	2629.85	6690.82	4234.39	59
H10B	2736.27	5194.86	2536.32	59
H12A	2163.97	6690.33	1882.44	61
H12B	2268.36	5186.73	186.68	61
H13A	1901.92	3321.22	1175.53	64
H13B	1797.48	4825.99	2867.46	64
H14A	1694.93	6684.21	-450.1	63
H14B	1798.51	5174.77	-2139.72	63
H2A	4451.2	6701.16	14163.27	66
H2B	4560.62	4926.76	15406.05	66
H15A	1330.28	4821.01	560.67	67
H15B	1433.44	3319.24	-1141.32	67
H17A	863.19	4814.93	-1703.93	73
H17B	964.81	3315.93	-3416.05	73

H16A	1225.09	6680.65	-2743.93	68
H16B	1327.21	5172.82	-4443.33	68
H18A	749.27	6669.12	-4998.12	76
H18B	852.42	5177.25	-6715.63	76
H19A	392.47	4771.46	-3945.71	95
H19B	495.02	3290	-5681.19	95
H20A	373.89	5145.37	-8953.7	146
H20B	270.94	6628.6	-7214.29	146
H20C	115.7	4773.84	-7464.03	146

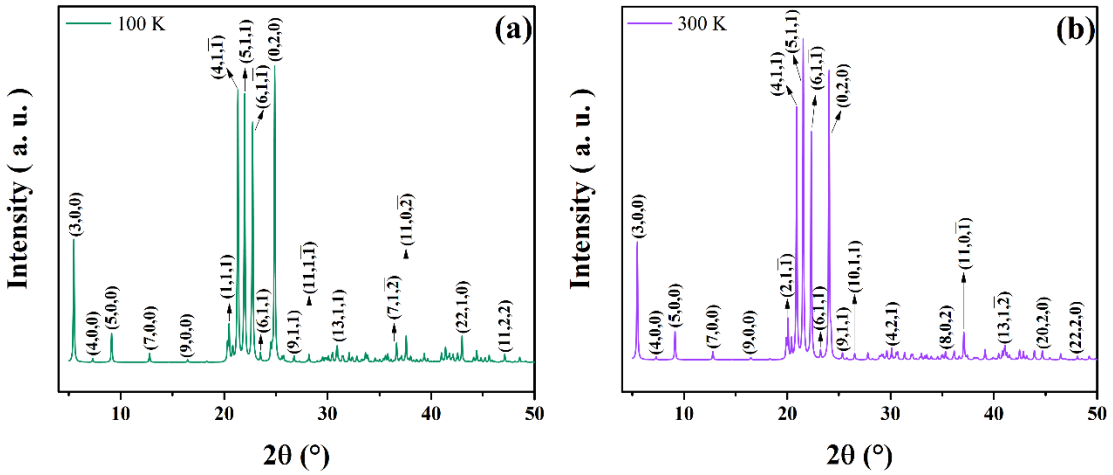

Figure S1. XRD patterns of AA single crystal in the B_m form at temperatures of (a) 100 K and (b) 300 K.

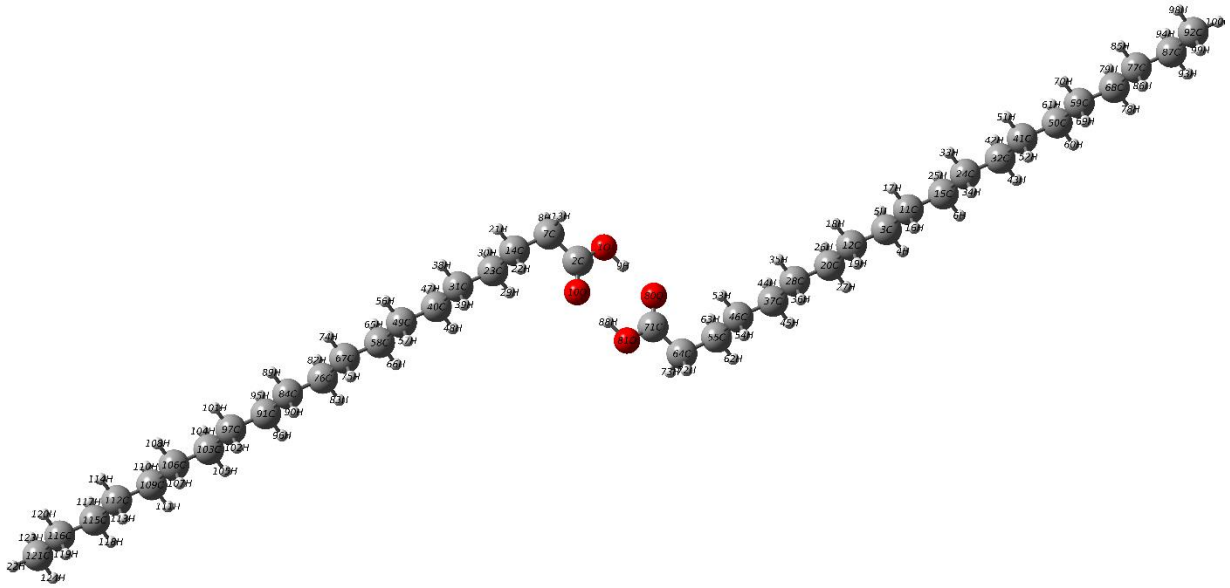

Figure S2. Dimer model for a pair of AA molecules used in the DFT calculations to obtain all intramolecular Raman-active modes. The gray and light gray balls represent carbon and hydrogen atoms, respectively. The red balls represent oxygen atoms.