

Table S10 – Structural and energetic parameters of L-LA trimer calculated at B3LYP/6-311++G(d,p) level of theory.

Dihedral / °	I-Tri	II-Tri	III-Tri	IV-Tri	V-Tri	VI-Tri	VII-Tri	VIII-Tri	IX-Tri	X-Tri	XI-Tri	XII-Tri	XIII-Tri	XIV-Tri	XV-Tri	XVI-Tri	XVII-Tri	XVIII-Tri
H _A -O ₉ -C ₃ -C ₁ ^a	-6.8	-56.6	14.8	16.2	1.5	-7.6	-43.5	-48.2	48.2	-93.8	-156.7	40.4	-43.3	164.1	164.0	171.4	172.8	-56.5
O _A -C ₃ -C ₁ =O	2.1	125.2	-14.2	-10.6	-3.3	4.8	-158.0	134.3	147.4	96.1	120.2	-32.2	-159.3	-32.6	-26.7	-19.6	148.8	124.9
O=C ₁ -O ₁₅ -C ₁₂	0.4	-9.4	-2.6	0.9	5.4	-0.6	3.7	-8.9	-4.2	-4.8	-9.4	-1.0	0.2	3.8	-3.5	-0.7	-3.2	-8.5
C ₁ -O ₁₅ -C ₁₂ -C ₁₃	-128.1	-68.9	-87.7	-72.6	-75.9	-73.1	-76.7	-71.7	-91.4	-74.6	-74.9	-87.4	-70.8	-75.7	-91.7	-79.2	-84.2	-65.1
O ₁₅ -C ₁₂ -C ₁₃ =O	-154.5	167.8	167.5	165.7	-171.4	166.2	-169.1	168.0	180.0	162.8	164.3	174.4	162.9	-170.5	163.2	162.5	168.1	162.6
O=C ₁₃ -O _E -C ₂₁	-4.0	-6.4	0.0	-3.0	-3.4	-4.4	-3.8	-4.0	-1.2	-0.6	-1.0	8.2	6.8	-2.6	-2.4	-1.2	-1.5	-7.0
C ₁₃ -O _E -C ₂₁ -C ₂₃	-76.4	-143.5	-78.3	-139.1	-118.5	-136.5	-132.6	-148.9	-80.5	-153.9	-155.5	-82.4	-81.6	-130.0	-79.7	-78.2	-83.8	-142.5
O _E -C ₂₁ -C ₂₃ =O	-9.0	-13.0	169.2	-5.9	-174.1	-171.8	-166.6	173.3	175.2	176.0	177.2	-115.5	-114.4	-167.9	-13.5	168.3	174.7	-12.8
O=C ₂₃ -O ₂₈ -H _C	0.2	-0.1	-2.5	0.2	178.0	-1.5	178.1	-0.9	-1.8	-179.9	-179.6	179.6	178.0	178.3	0.6	-3.3	-2.2	176.6
$\Delta E^{ZPE} / \text{kJ mol}^{-1}$	0.0	1.5	1.9	2.0	2.1	3.1	7.5	9.3	10.6	12.4	12.5	12.6	15.4	20.1	21.4	22.1	25.0	26.9

^a See **Fig. S2** for atom labeling. **I-Tri** – SSSSK'ASG'SC; **II-Tri** – G'SKSG'ASSK'SC; **III-Tri** – SSSG'ASG'AC; **IV-Tri** – SSSG'ASSK'SC; **V-Tri** – SSSG'ASSK'AT; **VI-Tri** – SSSG'ASSK'AC; **VII-Tri** – G'ASG'ASSK'AT; **VIII-Tri** – G'SKSG'ASSK'AC; **IX-Tri** – GSKSSK'ASG'AC; **X-Tri** – SK'SKSG'ASSK'AT; **XI-Tri** – ASKSG'ASAAT; **XII-Tri** – GG'SG'ASG'SK'T; **XIII-Tri** – G'ASG'ASG'SK'T; **XIV-Tri** – AG'SG'ASSK'AT; **XV-Tri** – ASSSK'ASG'SC; **XVI-Tri** – ASSG'ASG'AC; **XVII-Tri** – ASKSG'ASG'AC; **XVIII-Tri** – G'SKSG'ASSK'ST.