

Supporting Information

Table S1. Summary of X-ray Crystallography Data of **L⁵Li**

Emp. Formula	C ₁₄ H ₁₂ NOSLi
Form. Weight	249.25
Crystal system	Cubic
Space group	I-43d
a (Å)	25.6289(2)
b (Å)	25.6289(2)
c (Å)	25.6289(2)
α(°)	90°
β(°)	90°
γ(°)	90°
Volume (Å ³)	16834.1(2)
Z	48
Density	1.180 Mg/m ³
F(000)	6240
Crystal size(mm ³)	0.50 x 0.45 x 0.40
• • range	2.97 to 25.98°
Index ranges	-17<=h<=31 -31<=k<=31 -29<=l<=17
Ref. collected	11277
Ind. Reflections	2612 [R(int) = 0.0363]
Complete to θ	99.8%
Max. and min transmission	1.000000 and 0.78818
Data / Restraints/ parameters	2612 / 0 / 165
GOF	1.175
Final R indices	R1=0.0819
[I > 2 sigma (I)]	wR2=0.2554
R indices	R1 = 0.0936
(all data)	wR2 = 0.2681
Largest diff. Peak and hole	0.661 and -0.687 e.Å ⁻³
Temperature	110(2) K
Wavelength	0.71073 Å
Abs. correction	SADABS
Refine. Method	Full-matrix least-squares on F ²

^aR1=|(F_o-|F_c)/|F_o||.

$${}^bR2 = \{[w(F_o^2 - F_c^2)^2] / [w](F_o^2)^2\}^{1/2}, w = 0.10.$$

$${}^cGoF = [w(F_o^2 - F_c^2)^2] / (N_{\text{reflms}} - N_{\text{params}})^{1/2}.$$

Table S2 Selected bond lengths (Å) and angle (°) of **L⁵Li**

	bond lengths (Å)
Li-O(1)	1.932(10)
Li-O(1B)	1.979(10)
Li-O(1C)	1.995(10)
Li-S(1)	2.825(10)
Li-N(1)	2.160(10)
	bond angle (°)
O(1B)-Li-N(1)	154.0(5)
O(1)-Li-O(1C)	92.0(4)
O(1)-Li-S(1)	143.6(5)
O(1C)-Li-S(1)	123.3(4)

Table S3. Summary of X-ray Crystallography Data of L^4Na

Emp. Formula	$C_{128}H_{128}N_8O_{20}Na_8$
Form. Weight	2282.30
Crystal system	Triclinic
Space group	P-1
a (Å)	12.3496(2)
b (Å)	22.1400(5)
c (Å)	24.1563(5)
α (°)	94.865(2)°
β (°)	98.374(2)°
γ (°)	99.712(2)°
Volume (Å ³)	6400.1(2)
Z	2
Density	1.184 Mg/m ³
F(000)	2400
Crystal size(mm ³)	0.40 x 0.40 x 0.20
• • range	2.82 to 26.00°
Index ranges	-15 ≤ h ≤ 15 -27 ≤ k ≤ 27 -29 ≤ l ≤ 29
Ref. collected	64094
Ind. Reflections	25131 [R(int) = 0.0294]
Complete to θ	99.9%
Max. and min transmission	1.000000 and 0.96375
Data / Restraints/ parameters	25131 / 0 / 1481
GOF	1.018
Final R indices	R1=0.0527
[I > 2 sigma (I)]	wR2=0.1781
R indices	R1 = 0.0776
(all data)	wR2 = 0.1878
Largest diff. Peak and hole	0.482 and -0.520 e.Å ⁻³
Temperature	110(2) K
Wavelength	0.71073 Å
Abs. correction	SADABS
Refine. Method	Full-matrix least-squares on F ²

$$^a R1 = \frac{|(F_o - F_c)|}{|F_o|}$$

$$^b R2 = \left\{ \frac{[w(F_o^2 - F_c^2)^2]}{[w](F_o^2)^2} \right\}^{1/2}, w = 0.10.$$

$$^c GoF = \left[\frac{[w(F_o^2 - F_c^2)^2]}{(N_{\text{rflns}} - N_{\text{params}})} \right]^{1/2}.$$

Table S4 Selected bond lengths (Å) and angle (°) of L⁴Na

	bond lengths (Å)
Na-O(1)	2.239(2)
Na-N(1)	2.383(2)
Na-O(2)	2.338(2)
Na-O(3)	2.328(2)
Na-O(7)	2.308(2)
Na-N(2)	2.897(3)
	bond angle (°)
O(2)-Na(1)-O(1)	150.05(9)
O(1)-Na(2)-O(9)	170.54(9)
N(2)-Na(1)-N(1)	84.71(8)
O(3)-Na(1)-N(2)	65.42(7)
O(3)-Na(1)-O(7)	86.45(7)
O(7)-Na(1)-N(1)	124.52(9)
O(4)-Na(2)-N(2)	65.29(8)
N(2)-Na(2)-O(3)	72.40(8)
O(3)-Na(2)-O(5)	85.03(7)
O(5)-Na(2)-O(4)	137.93(8)