Efficient Blue Light-Emitting Diodes Based on A classical "Push-Pull" Architecture Molecule 4,4'-di-(2-(2,5-dimethoxyphenyl)ethenyl)-2,2'-Bipyridine

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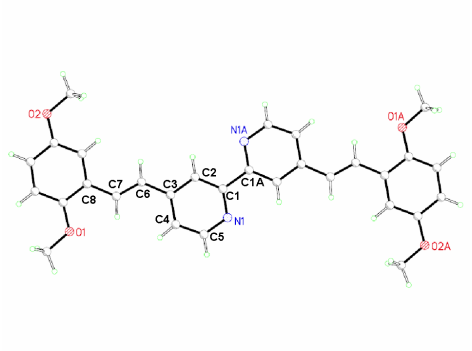
Supporting Information

Crystal data and structure refinement for N945L.

Identification code	N945L	
Empirical formula	C30 H28 N2 O4	
Formula weight	480.54	
Temperature	140(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.6670(8) Å	α= 90°.
	b = 13.7182(13) Å	β= 99.379(7)°.
	c = 11.7334(8) Å	γ = 90°.
Volume	1217.60(19) $Å^3$	
Z	2	
Density (calculated)	1.311 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	508	
Crystal size	0.14 x 0.12 x 0.08 mm^3	
Theta range for data collection	3.08 to 25.02°.	
Index ranges	-9<=h<=8, -16<=k<=16, -13<=l<=13	
Reflections collected	7148	
Independent reflections	2091 [R(int) = 0.0426]	
Completeness to theta = 25.02°	97.4 %	
Absorption correction	Semi-empirical from equivalents (MULABS)	
Max. and min. transmission	0.9974 and 0.9588	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2091 / 0 / 163	
Goodness-of-fit on F^2	0.865	
Final R indices [I>2sigma(I)]	R1 = 0.0349, wR2 = 0.0630	
R indices (all data)	R1 = 0.0873, wR2 = 0.0740	
Largest diff. peak and hole	0.145 and -0.133 $e.Å^{-3}$	

Table S1: Comparison between main optimized geometrical parameters (Å, º) and X-ray data for the N945L ligand.



Parameter	X-ray	Theor. (2-5)	Theor. (3-4)
$d_{(C1-C1A)}$	1.494	1.491	1.491
$d_{(C1-C2)}$	1.386	1.399	1.400
$d_{(C2-C3)}$	1.396	1.403	1.403
$d_{(C1-N1)}$	1.350	1.345	1.345
$d_{(N1-C5)}$	1.349	1.338	1.338
$d_{(C4-C5)}$	1.375	1.390	1.390
$d_{(C3-C4)}$	1.400	1.408	1.408
$d_{(C3-C6)}$	1.466	1.464	1.464
$d_{(C6-C7)}$	1.334	1.350	1.350
$d_{(C7-C8)}$	1.463	1.463	1.436
$a_{(C1A-C1-N1)}$	116.4	117.0	117.0
$a_{(C1A-C1-C2)}$	121.2	120.5	120.5
$a_{(C1-N1-C5)}$	116.3	117.2	117.2
$a_{(C1-C2-C3)}$	121.1	120.3	120.3
$a_{(C2-C3-C6)}$	120.0	119.3	119.1
$a_{(C3-C6-C7)}$	126.7	126.1	126.4
$a_{(C6-C7-C8)}$	127.3	126.6	127.4

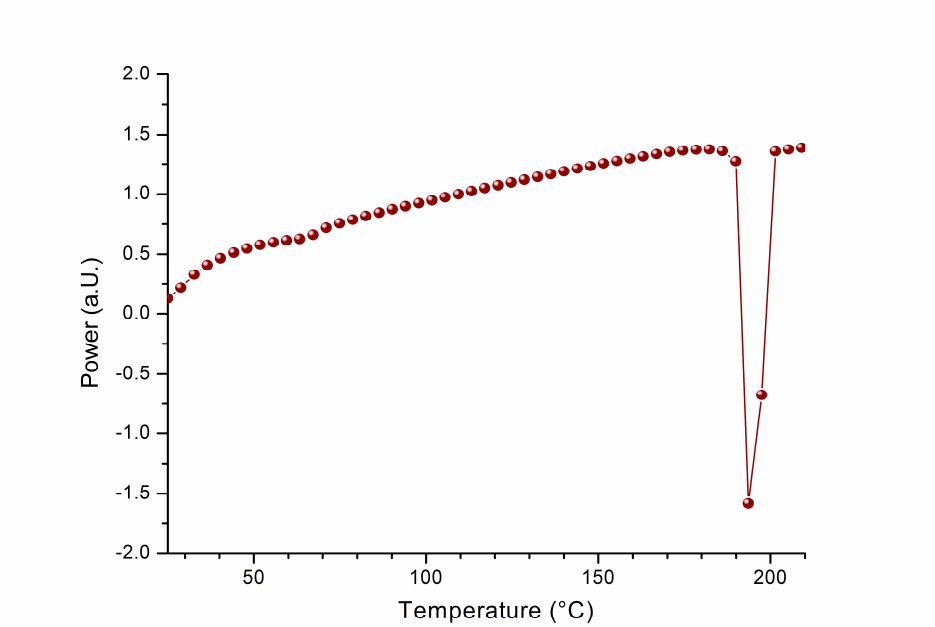


Figure S1: Differential scanning calorimeter trace of N945L.

Reference [24]: R. B. Gaussian 03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J., *Gaussian, Inc.: Pittsburgh PA* **2003**.