Supporting Information

for

High Solid-State Luminescence in Propeller-Shaped AIE-active Pyridine-Ketoiminate-Boron Complexes

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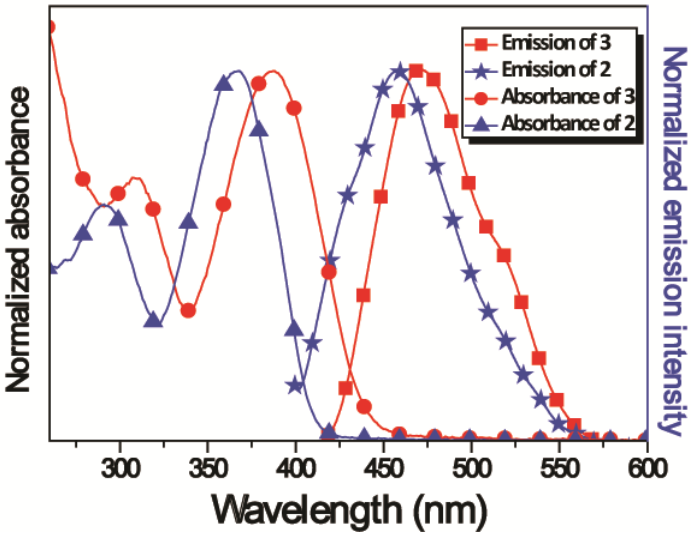

Figure S1. Absorption and emission spectra of **2** and **3** in dichloromethane (50 μM).

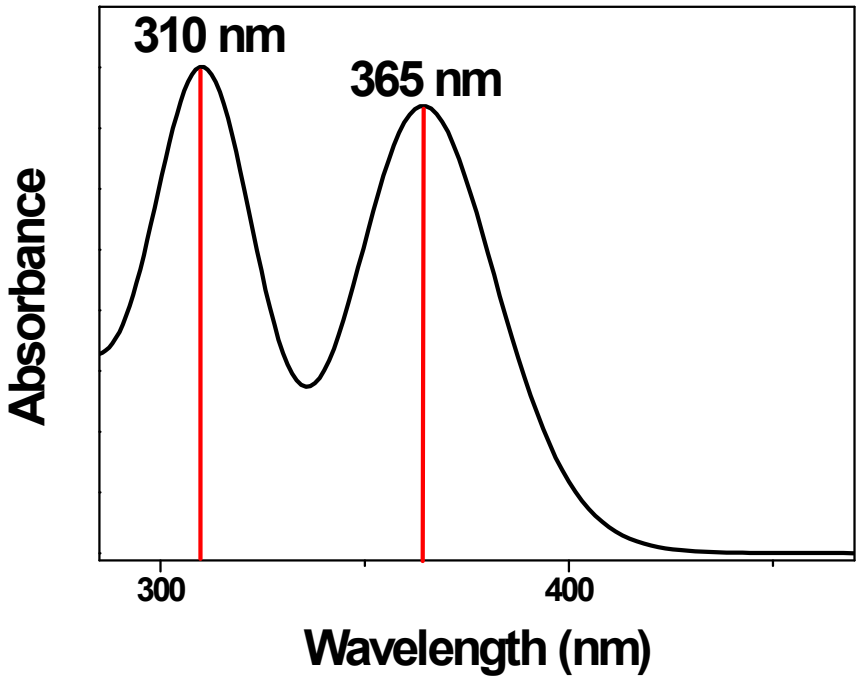

Figure S2. Calculated absorption spectra of **2**.

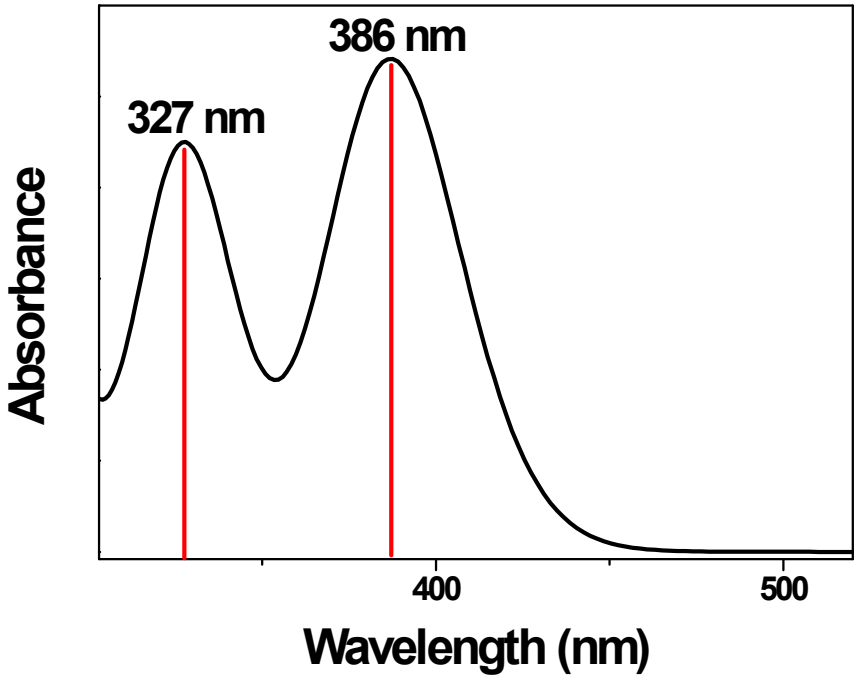

Figure S3. Calculated absorption spectra of **3**.

Table S1. Crystal data and structure refinement for **2**.

Identification code	**2**
Empirical formula	C19H14BF2NO
Formula weight	321.12
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 10.2403(9) Å α = 90°
	b = 12.1323(11) Å β =92.5160°
	c = 12.4975(12) Å γ=90°
Volume	1551.2(2) $Å^3$
Z, Calculated density	4, 1.375 Mg/m^3
Absorption coefficient	0.100 mm^{-1}
F(000)	664
Crystal size	0.45 x 0.43 x 0.42 mm^3
Theta range for data collection	2.34 to 25.02°
Limiting indices	-10<=h<=12, -9<=k<=14, -13<=l<=14
Reflections collected / unique	7566 / 2735 [R(int) = 0.0456]
Completeness to theta = 25.02	99.8 %
Absorption correction	None
Max. and min. transmission	0.9857 and 0.9690
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2735 / 0 / 218
Goodness-of-fit on F^2	0.960
Final R indices [I>2σ(I)]	R1 = 0.0379, wR2 = 0.0920
R indices (all data)	R1 = 0.0739, wR2 = 0.1122
Extinction coefficient	0.061(4)
Largest diff. peak and hole	0.134 and -0.155 $e.Å^{-3}$

Table S2. Crystal data and structure refinement for **3**.

Identification code	**3**
Empirical formula	C31H24BNO
Formula weight	437.32
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.2542(8)Å α = 109.354(2)°
	b = 9.8875(9)Å β = 102.8820(10)°
	c = 14.4448(13)Å γ= 95.3860(10)°
Volume	1195.24(18)Å^3
Z, Calculated density	2, 1.215 Mg/m^3
Absorption coefficient	0.072 mm^{-1}
F(000)	460
Crystal size	0.44 x 0.37 x 0.20 mm^3
Theta range for data collection	2.89 to 25.02°
Limiting indices	-10<=h<=10, -11<=k<=11, -14<=l<=17
Reflections collected / unique	5993 / 4122 [R(int) = 0.0271]
Completeness to theta = 25.02	98.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9857 and 0.9690
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4122 / 0 / 307
Goodness-of-fit on F^2	0.697
Final R indices [I>2σ(I)]	R1 = 0.0511, wR2 = 0.1568
R indices (all data)	R1 = 0.1048, wR2 = 0.2173
Largest diff. peak and hole	0.206 and -0.192 e.Å^{-3}

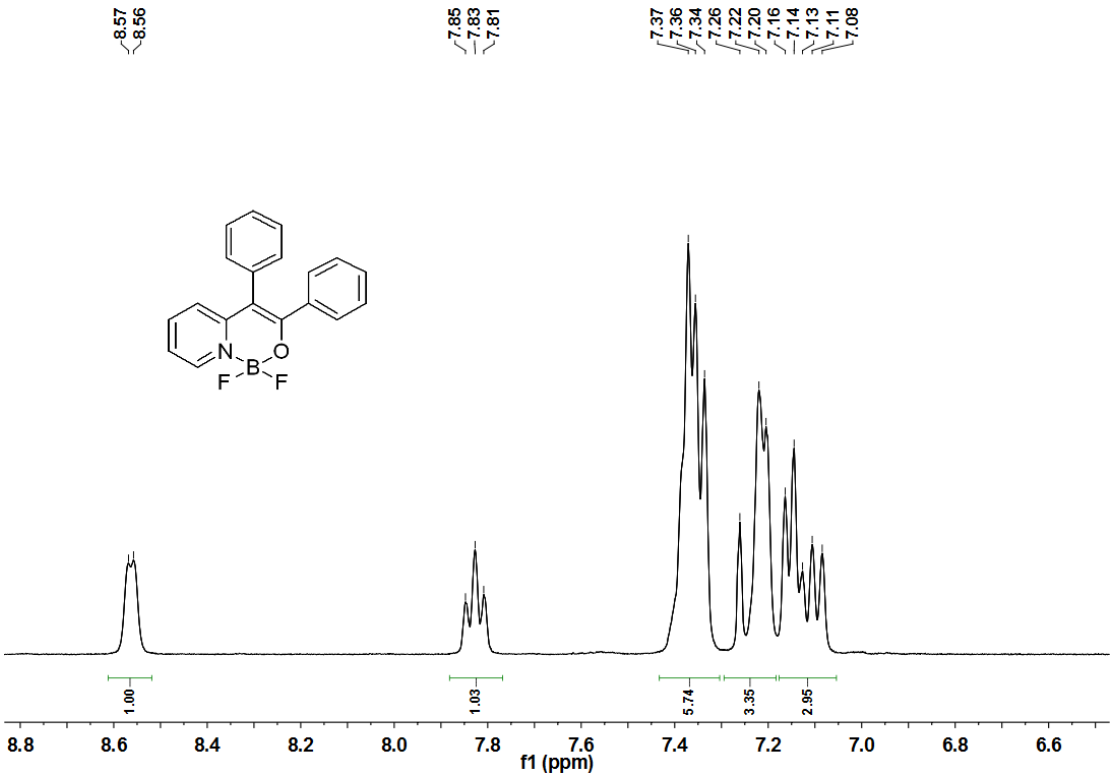

Figure S4. ^{1}H NMR spectrum of **2** in $CDCl_3$.

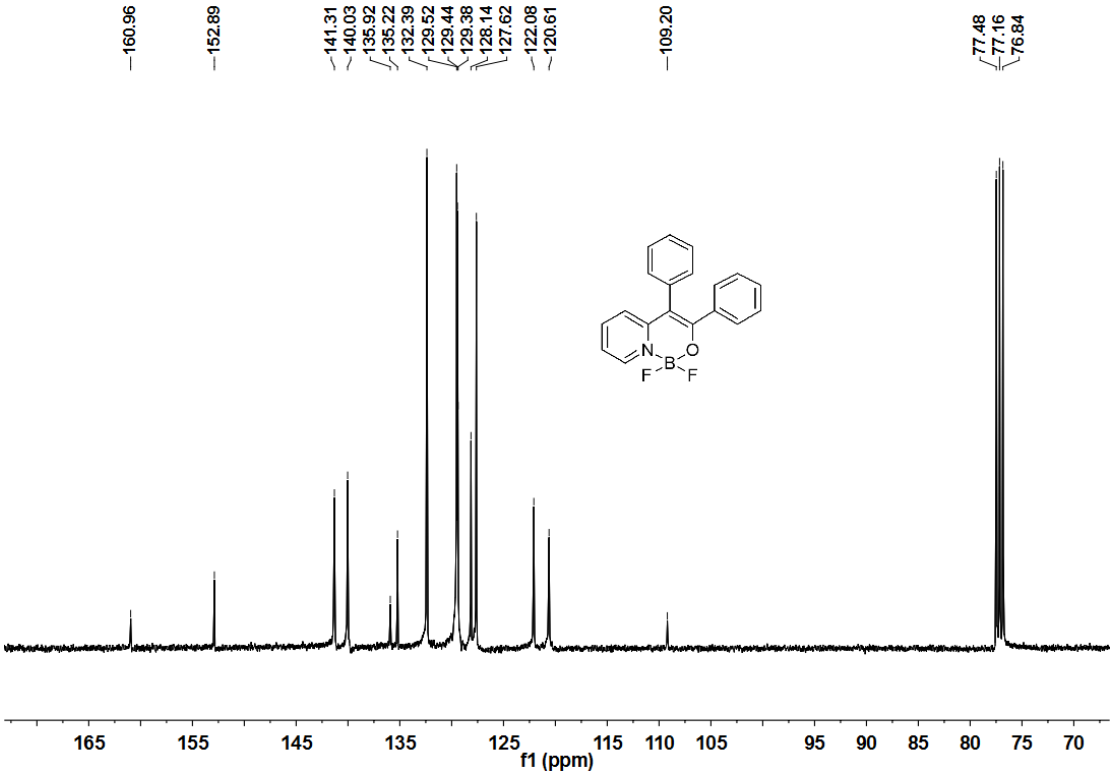

Figure S5. ^{13}C NMR spectrum of **2** in $CDCl_3$.

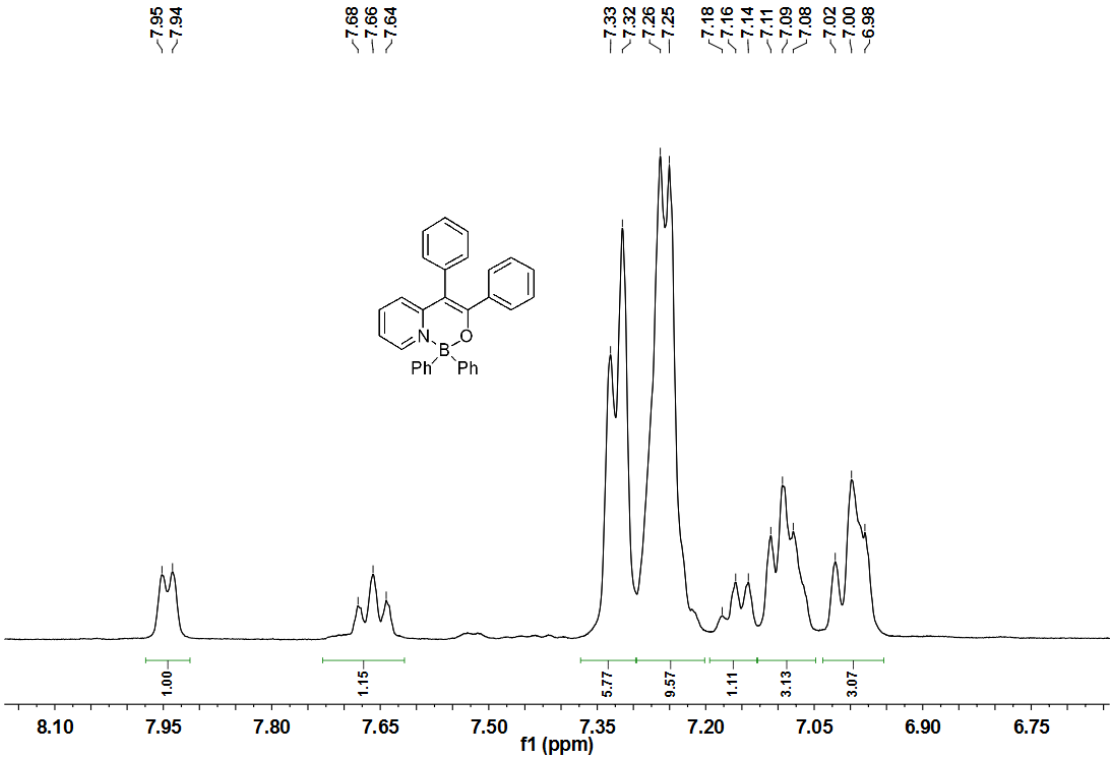

Figure S6. ^{1}H NMR spectrum of **3** in $CDCl_3$.

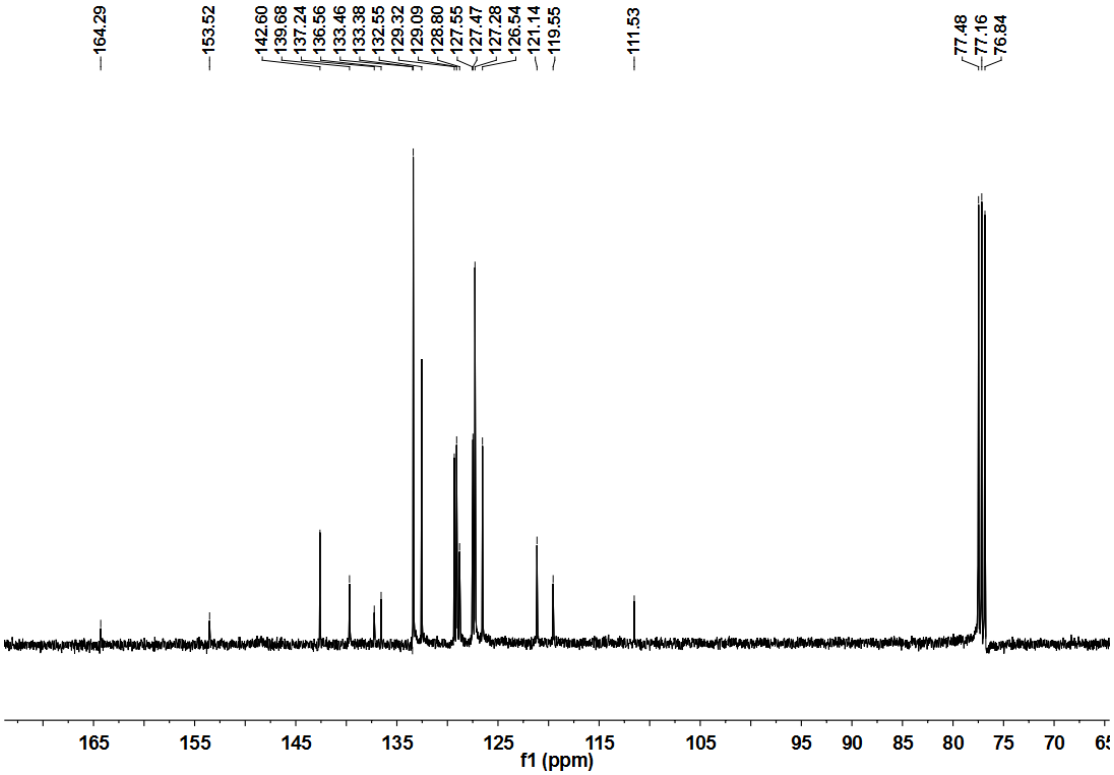

Figure S7. ^{13}C NMR spectrum of **3** in $CDCl_3$.

Z-matrix and total energy of **2**

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

F	-2.3138	7.9531	12.5652
F	-1.8578	8.9599	10.605
N	-1.3178	6.6575	10.8028
O	-0.1234	8.3977	12.0393
B	-1.4161	8.0442	11.5319
C	-2.4245	5.9018	10.6807
H	-3.2038	6.1766	11.1071
C	-2.4446	4.7502	9.9568
H	-3.2144	4.2317	9.9047
C	-1.2894	4.3737	9.3023
H	-1.2789	3.6021	8.7835
C	-0.1632	5.135	9.4177
H	0.6077	4.8845	8.9621
C	-0.1495	6.2867	10.2102
C	1.0357	7.09	10.4593
C	1.0121	8.0611	11.4083
C	2.1662	8.8338	11.9312
C	1.9485	10.117	12.4039
H	1.0981	10.4884	12.3444
C	2.9716	10.8536	12.9603
H	2.809	11.7198	13.2596
C	4.2282	10.3173	13.0748
H	4.9147	10.8111	13.4606
C	4.4645	9.0483	12.6152
H	5.3176	8.6843	12.6827
C	3.4478	8.3042	12.0526
H	3.6207	7.4407	11.7513
C	2.2765	6.7553	9.7041
C	2.954	5.5692	9.9203
H	2.6135	4.9548	10.5302
C	4.1228	5.2794	9.2511
H	4.5653	4.4768	9.4103
C	4.6305	6.1802	8.3473
H	5.4234	5.9909	7.8983
C	3.9713	7.3582	8.1066
H	4.3167	7.9661	7.4938
C	2.7957	7.6436	8.7722
H	2.3473	8.4392	8.595

Total Energy, E(TD-HF/TD-KS) = -1086.79494656

Z-matrix and total energy of **3**.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-1.4399	-1.05	10.9776
N	-2.8716	-1.8875	9.1675
C	-2.2739	-0.0237	11.1753
C	-3.7873	-0.9349	9.4967
C	-3.4058	0.1209	10.4125
C	-1.849	0.855	12.2979
C	-0.7107	-0.5347	8.5809
C	-0.5628	-3.0332	9.7079
C	-2.7257	1.5538	13.1219
H	-3.6406	1.5044	12.9631
C	-4.3063	1.3161	10.5284
C	-4.4802	-3.098	7.8933
H	-4.7012	-3.8411	7.3803
C	-0.4898	0.9241	12.5905
H	0.1168	0.4513	12.0683
C	-3.2137	-2.9324	8.3906
H	-2.566	-3.5673	8.1833
C	-5.5645	1.2503	11.1066
H	-5.8777	0.4355	11.4293
C	-5.0696	-1.0608	8.9509
H	-5.7014	-0.4003	9.1227
C	-0.9021	2.3849	14.4326
H	-0.5861	2.9028	15.1372
C	0.5353	0.0248	8.8551
H	1.0015	-0.2666	9.6056
C	-3.8668	2.5349	10.0556
H	-3.0288	2.6012	9.6581
C	-5.418	-2.1265	8.1767
H	-6.2816	-2.1985	7.8409
C	-0.7191	-3.8604	10.8205
H	-1.231	-3.5588	11.5369
C	-0.0324	1.6816	13.6454
H	0.8798	1.7149	13.8252
C	-2.2603	2.3154	14.1663
H	-2.86	2.7866	14.6977
C	-1.3496	-0.0668	7.4354
H	-2.1784	-0.4208	7.2045
B	-1.3319	-1.6279	9.603

C	-0.7854	0.9125	6.6272
H	-1.2447	1.2123	5.8754
C	1.1071	0.9972	8.0547
H	1.9389	1.3504	8.2752
C	0.4455	1.4427	6.9316
H	0.8266	2.0928	6.3871
C	0.2251	-3.546	8.6845
H	0.3623	-3.0261	7.9261
C	-6.3581	2.3705	11.2129
H	-7.1966	2.3155	11.6117
C	0.816	-4.802	8.7449
H	1.3381	-5.1058	8.039
C	0.6278	-5.5927	9.8496
H	1.0119	-6.4384	9.8929
C	-4.6583	3.6535	10.1685
H	-4.3435	4.4739	9.8641
C	-0.1387	-5.1206	10.8966
H	-0.2654	-5.6463	11.6524
C	-5.8996	3.5697	10.7221
H	-6.4386	4.326	10.7694

Total Energy, E(TD-HF/TD-KS) = -1350.09452917