

Supplementary Information

Triazatruxene Decorated Multi-Resonance Emitter with Hybrid Short- and Long-Range Charge-Transfer Excited States Enabled Efficient Deep-Blue Electroluminescence

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Table of contents

General information	3
Quantum Chemical Calculations	3
Analysis of Rate Constants:	4
Device Fabrication and Characterization	4
Synthesis of the Materials	5
Thermal and Electrochemical Properties	8
Theoretical Calculation	10
Photophysical Properties	11
Electroluminescence Devices	12
References	15
Cartesian Coordinates	15

General information

Unless otherwise indicated, all starting materials were obtained from commercial suppliers and were used without further purification. All the reaction solvents were purified by solvent purification system prior to use.

The ^1H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded in deuterated chloroform (CDCl_3) solution on Bruker NMR spectrometer with tetramethylsilane (TMS, δ 0.00) as the internal standard. High-resolution electrospray (ESI) mass spectra were performed on SCIEX TripleTOF6600 nanoLCMS. Thermogravimetric analysis (TGA) was undertaken using a PerkinElmer Instruments (Pyris1 TGA) at a heating rate of $10\text{ }^\circ\text{C}/\text{min}$ from 30 to $800\text{ }^\circ\text{C}$ under a nitrogen environment. UV-vis absorption spectra were recorded on a Shimadzu UV-2700 recording spectrophotometer. Photoluminescence (PL) spectra were recorded on a Hitachi F-4600 fluorescence spectrophotometer. The lifetimes of fluorescence and delayed fluorescence were performed on PicoQuant Fluotime300. Absolute PLQYs were obtained using a Quantaaurus-QY measurement system (C9920-02, Hamamatsu Photonics). Cyclic voltammetry (CV) was carried out in nitrogen-purged dichloromethane (oxidation scan) at room temperature with a CHI voltammetric analyzer. Tetrabutylammonium hexafluorophosphate (TBAPF_6) (0.1 M) was used as the supporting electrolyte. The conventional three-electrode configuration consists of a platinum working electrode, a platinum wire auxiliary electrode, and an Ag wire pseudo reference electrode with ferrocenium/ferrocene (Fc^+/Fc) as the internal standard. The intermediate 5,10-diphenyl-10,15-dihydro-5H-diindolo[3,2-*a*:3',2'-*c*]carbazole (**TAT2P**)^[1] and **BNO-Br**^[2] was synthesized according to the literature methods using commercially available raw materials.

Quantum Chemical Calculations

Theoretical chemical calculations were performed using the Gaussian 16 program package. S_0 geometries were obtained based on Density functional theory (DFT) with B3LYP-D3(BJ)/6-31G(d, p) method. Time-dependent DFT (TD-DFT) calculations were carried out by the same method to afford optimized S_1 geometry. To account for electron correlation through double excitations, higher-level mPW2PLYP calculations were performed to model the excited-state energy levels with the def2SVP basis set, using the ORCA program. Spin-orbit coupling (SOC) matrix element values between S_1 and T_n ($n = 1, 2, \dots$) states were computed using PySOC aligned with the TD-DFT settings. Franck-Condon analyses were performed according to the literature using the Gaussian 16 package and MOMAP within the DUSHIN module. All calculations were performed in the gas phase and visualized using GaussView 6.0 or VMD 1.9.3.^[3,4]

Analysis of Rate Constants:

The rate constants of radiative decay ($k_{r,S}$) and nonradiative decay ($k_{nr,S}$) from S_1 to S_0 states, the rate constants of intersystem crossing (k_{ISC}) and reverse intersystem crossing (k_{RISC}) were calculated from the following six equations: [5,6]

$$k_p = 1/\tau_p \dots\dots\dots (Eq.S1)$$

$$k_d = 1/\tau_d \dots\dots\dots (Eq.S2)$$

$$k_{r,S} = \Phi_p k_p + \Phi_d k_d \approx \Phi_p k_p \dots\dots\dots (Eq.S3)$$

$$k_{nr,S} = \frac{1 - \Phi_{PL}}{\Phi_{PL}} k_{r,S} \dots\dots\dots (Eq.S4)$$

$$k_{ISC} = k_p - k_{r,S} - k_{nr,S} \dots\dots\dots (Eq.S5)$$

$$k_{RISC} = (k_p k_d \Phi_d) / (k_{ISC} \Phi_p) \dots\dots\dots (Eq.S6)$$

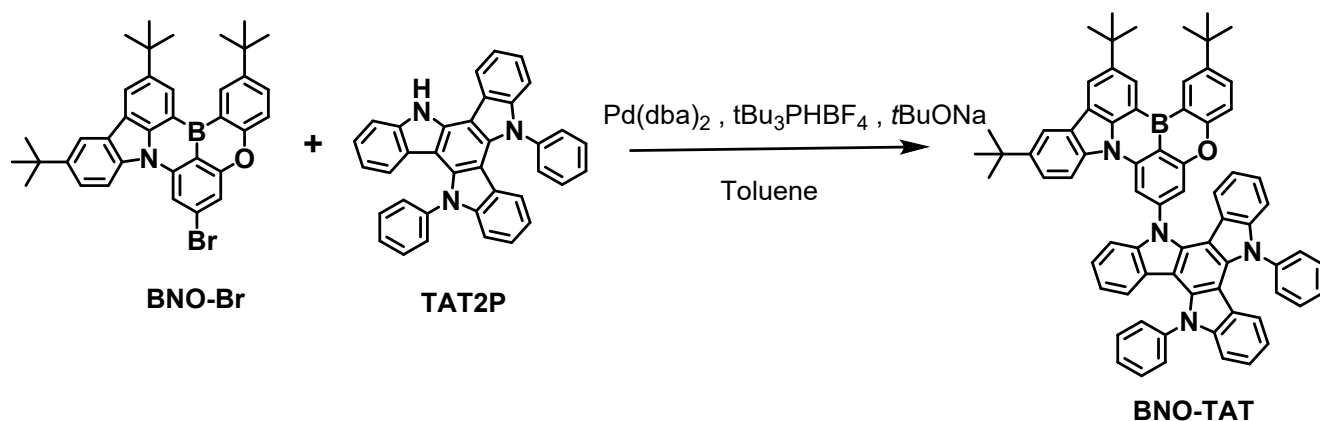
Where τ_p and τ_d represent the prompt and decay fluorescence lifetime, which determined from transient PL spectra. The k_p and k_d represent the decay rate constants for prompt and delayed fluorescence, respectively. Φ_p and Φ_d indicate prompt and delayed fluorescence components and can be distinguished from the total Φ_{PL} by comparing the integrated intensities of prompt and delayed components in the transient PL spectra.

Device Fabrication and Characterization

The ITO coated glass substrates with a sheet resistance of $15 \Omega \text{ square}^{-1}$ were consecutively ultrasonicated with acetone/ethanol and dried with nitrogen gas flow, followed by 20 min ultraviolet light-ozone (UVO) treatment in a UV-ozone surface processor (PL16 series, Sen Lights Corporation). Then the sample was transferred to the deposition system. Both 8-hydroxyquinolinolato-lithium (Liq) as electron injection layer and aluminum (Al) as cathode layer were deposited by thermal evaporation at 5×10^{-5} Pa. Additionally, the organic layers were deposited at the rates of 0.2-3 Å/s. After the organic film deposition, Liq and Al layer were deposited with rates of 0.1 and 3 Å/s, respectively. The emitting area of the device is about 0.09 cm². The current density-voltage-luminance (J - V - L), L-EQE curves and electroluminescence spectra were measured using a Keithley 2400 source meter and an absolute EQE measurement system (C9920-12, Hamamatsu Photonics, Japan). The doped films were fabricated by thermal evaporation of the organic emitters

at the rates of 0.2-3.0 Å s⁻¹, and the size of the quartz used for sample is 1 cm * 2 cm.

Synthesis of the Materials



Scheme S1. Synthesis of **BNO-TAT**

Synthesis of 2,11,14-tri-*tert*-butyl-7-(10,15-diphenyl-10,15-dihydro-5*H*-diindolo[3,2-*a*:3',2'-*c*]carbazol-5-yl)-5-oxa-8b-aza-15b-borabenz[*a*]naphtho[1,2,3-*hi*]aceanthrylene (**BNO-TAT**): **BNO-Br** (0.88 g, 1.5 mmol), **TAT2P** (0.82 g, 1.65 mmol), Pd(dba)₂ (115 mg), *t*Bu₃PHBF₄ (116 mg), and *t*BuONa (0.52 g, 5.4 mmol) were added into a 100 mL two neck flask. After that, 25 mL toluene was injected into the two-neck flask under argon atmosphere. The mixture was stirred at 110 °C for 12 h. After cooling to room temperature, the crude product was removed under vacuum and then purified by silica gel chromatography using petroleum ether/dichloromethane (4/1) as eluent to give the product **BNO-TAT** (1.00 g, 65%) as yellow powder. The powder was further purified by sublimation to afford the product as greenish yellow crystal. MS: MW 1006.48, *m/z* = 1007.48 [M+H]⁺. ¹H NMR (500 MHz, toluene-*d*₈) δ (ppm) 9.29 (d, *J* = 1.6 Hz, 1H), 9.19 (d, *J* = 2.5 Hz, 1H), 8.69 (d, *J* = 1.5 Hz, 1H), 8.52 (d, *J* = 1.6 Hz, 1H), 8.20 (d, *J* = 1.8 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.75 (d, *J* = 1.4 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.56 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.44 (br, 7H), 7.31 – 7.16 (m, 10H), 7.03 (br, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 6.81 (dd, *J* = 8.2, 7.0 Hz, 1H), 6.61 (dd, *J* = 8.2, 7.0 Hz, 1H), 6.51 – 6.44 (m, 2H), 1.66 (s, 9H), 1.52 (s, 9H), 1.33 (s, 9H). ¹³C NMR (126 MHz, toluene-*d*₈) δ 160.69, 158.31, 146.05, 145.16, 145.02, 144.74, 143.50, 142.57, 142.14, 142.03, 141.99, 141.30, 141.19, 138.20, 137.90, 137.80, 137.62, 131.14, 130.73, 129.76, 129.69, 129.65, 128.90, 126.94, 123.82, 123.74, 123.71, 123.50, 123.13, 122.98, 122.92, 122.79, 120.96, 120.88, 120.45, 120.32, 117.78, 116.76, 113.68, 110.37, 110.08, 110.06, 108.89, 107.79, 105.73, 105.71, 105.48, 34.93, 34.35, 34.33, 31.92, 31.37, 31.36. HRMS (ESI) *m/z* calculated for C₇₂H₆₀ON₄B [M+H]⁺ 1007.4855, found 1007.4829.

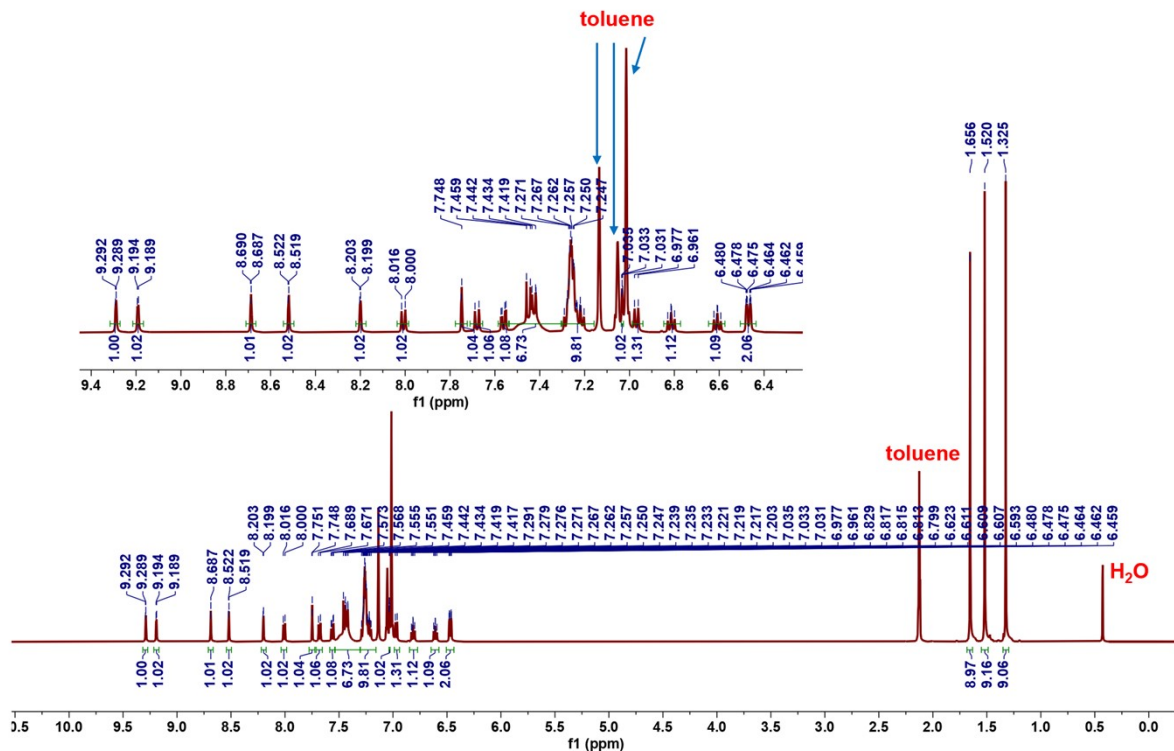


Fig. S1 ^1H NMR spectrum of BNO-TAT in $\text{toluene-}d_8$

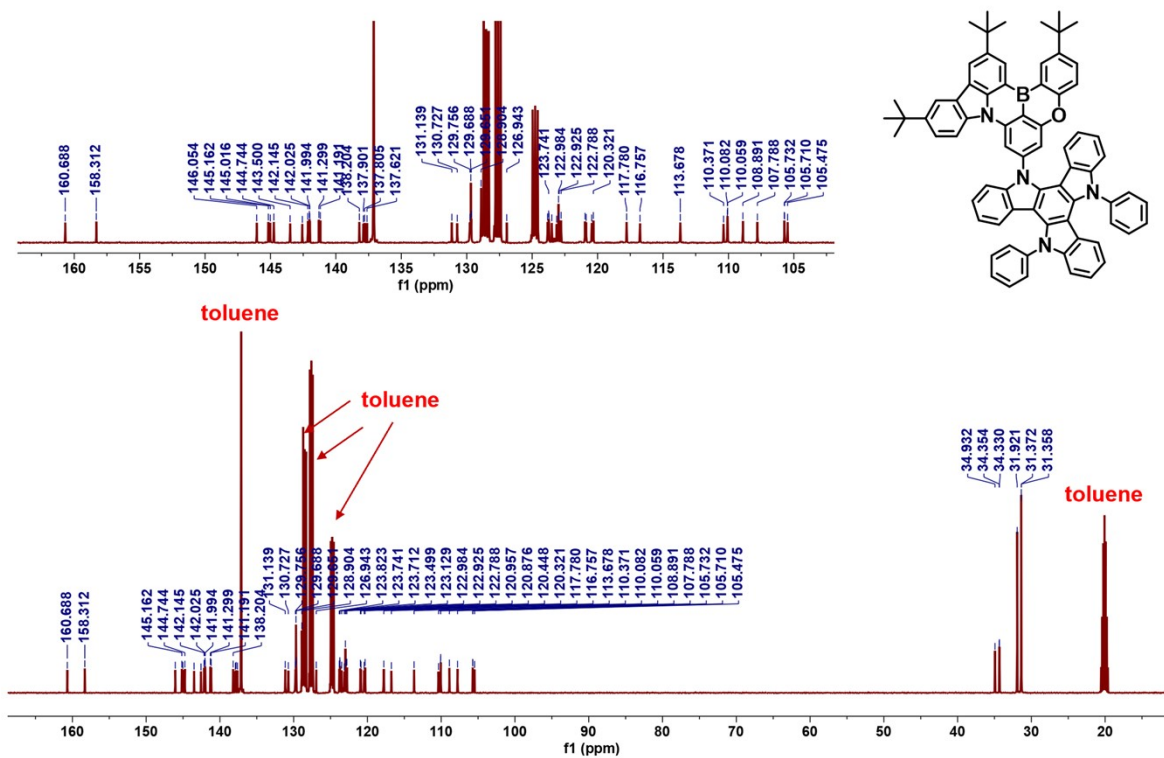


Fig. S2 ^{13}C NMR spectrum of BNO-TAT in $\text{toluene-}d_8$

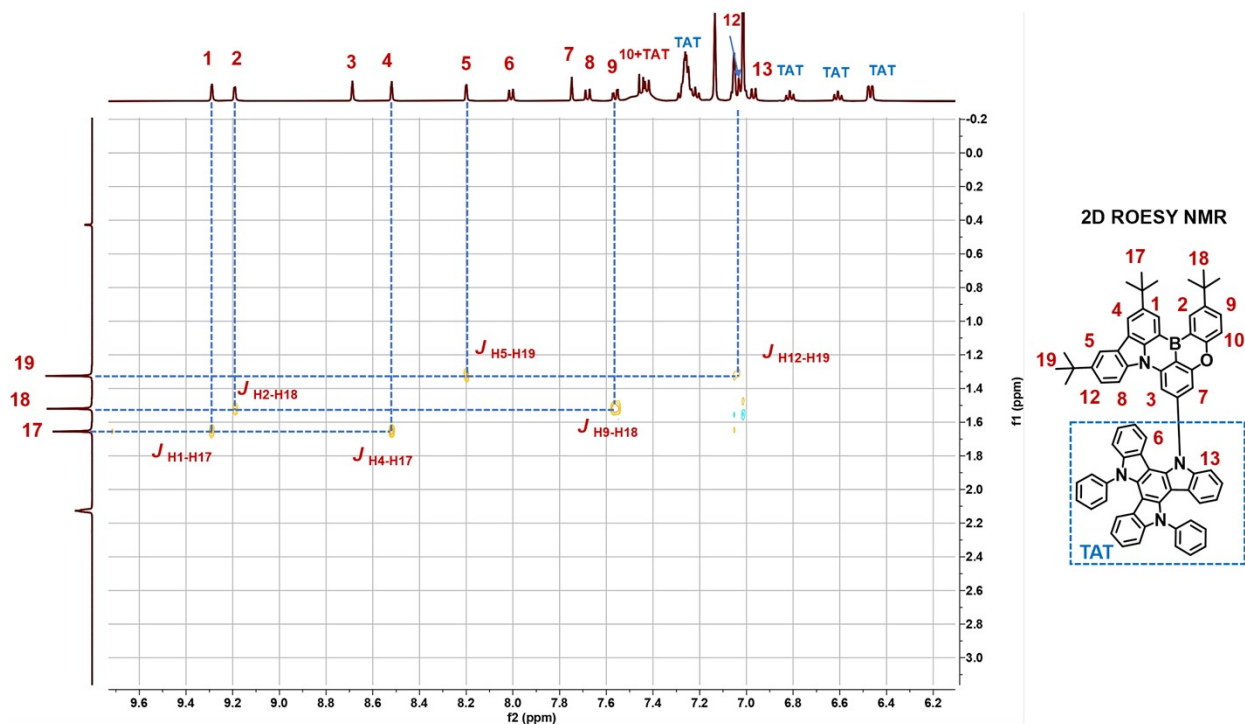


Fig. S5 2D ROESY NMR of BNO-TAT (high-field region) in toluene- d_8

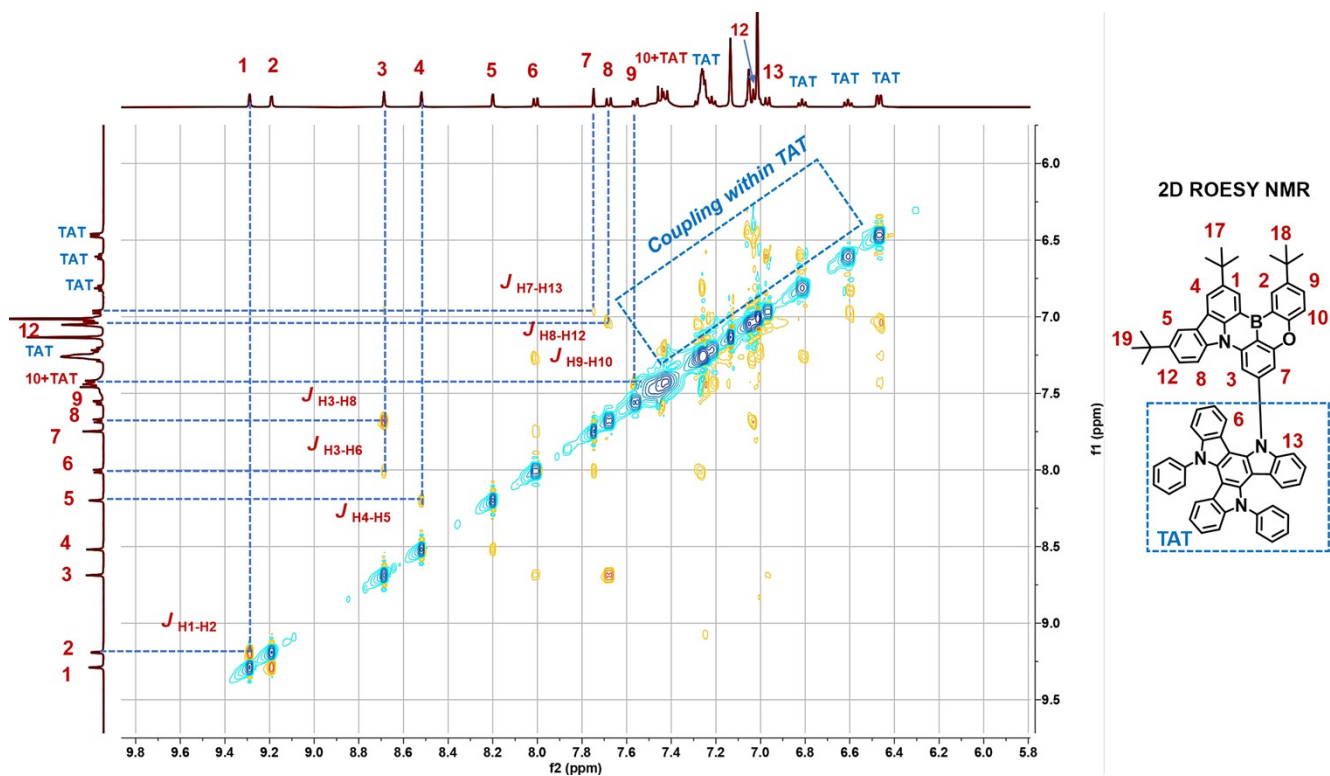


Fig. S6 2D ROESY NMR of BNO-TAT (aromatic region) in toluene- d_8

Thermal and Electrochemical Properties

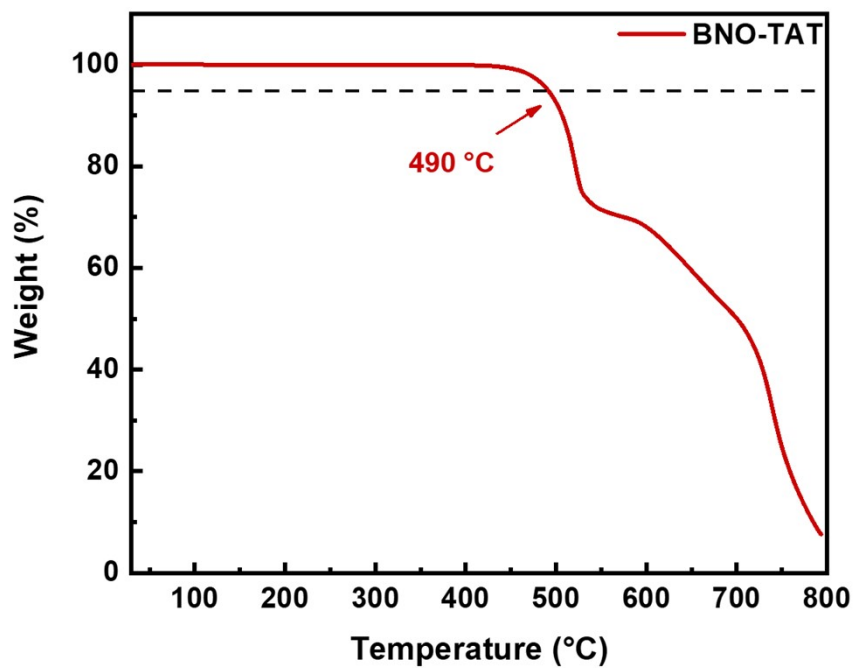


Fig. S7 Thermogravimetric analysis (TGA) curve of **BNO-TAT**

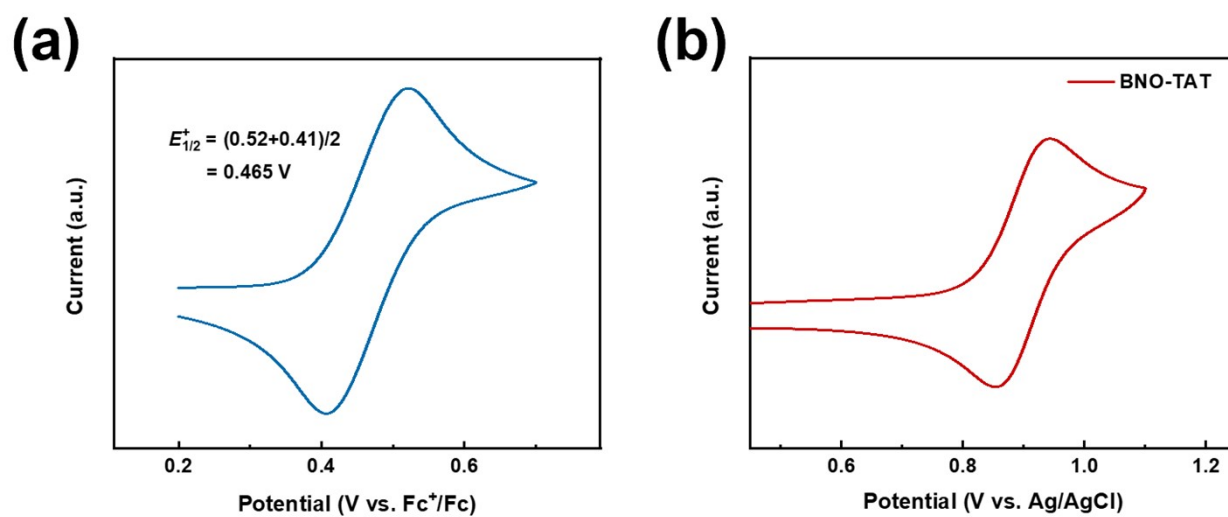


Fig. S8 Cyclic voltammograms (CV) of a) ferrocene/ferrocenium (Fc/Fc⁺) and b) **BNO-TAT**

Theoretical Calculation

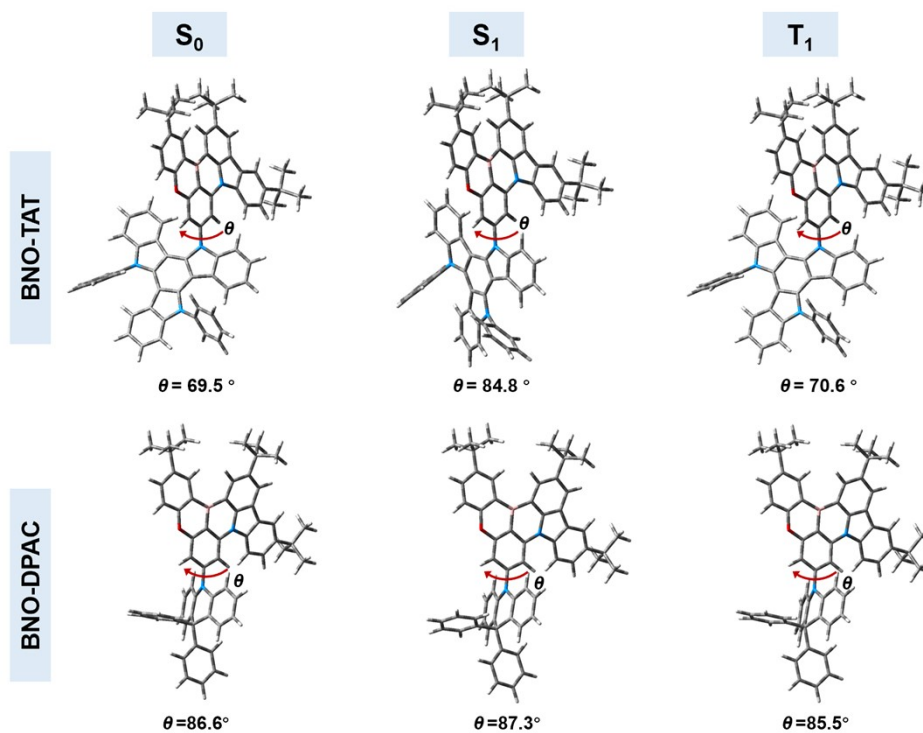


Fig. S9 The optimized geometries of BNO-DPAC and BNO-TAT at different states

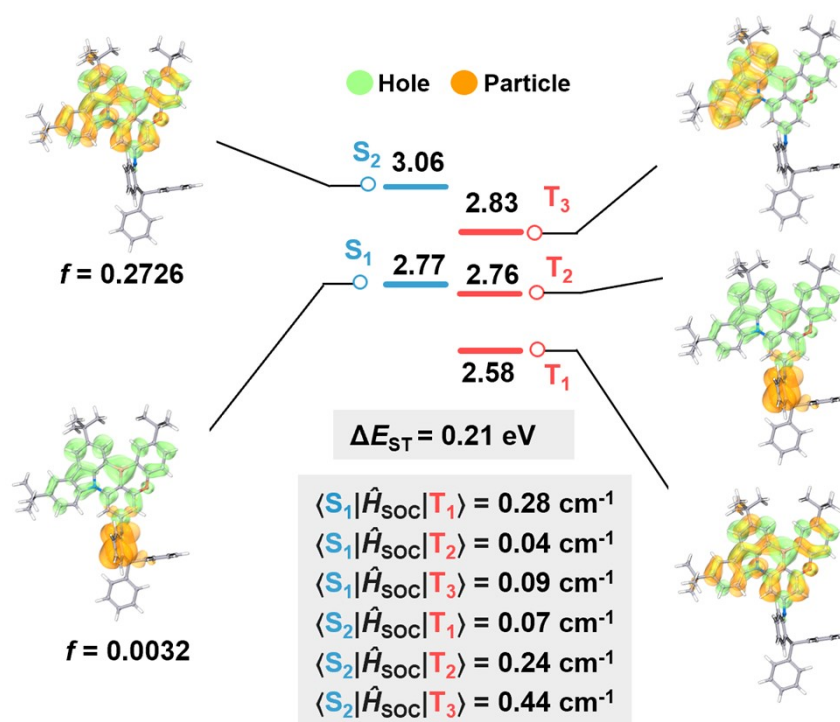


Fig. S10 Calculated state energy energies, NTO distributions and SOCMEs of BNO-DPAC

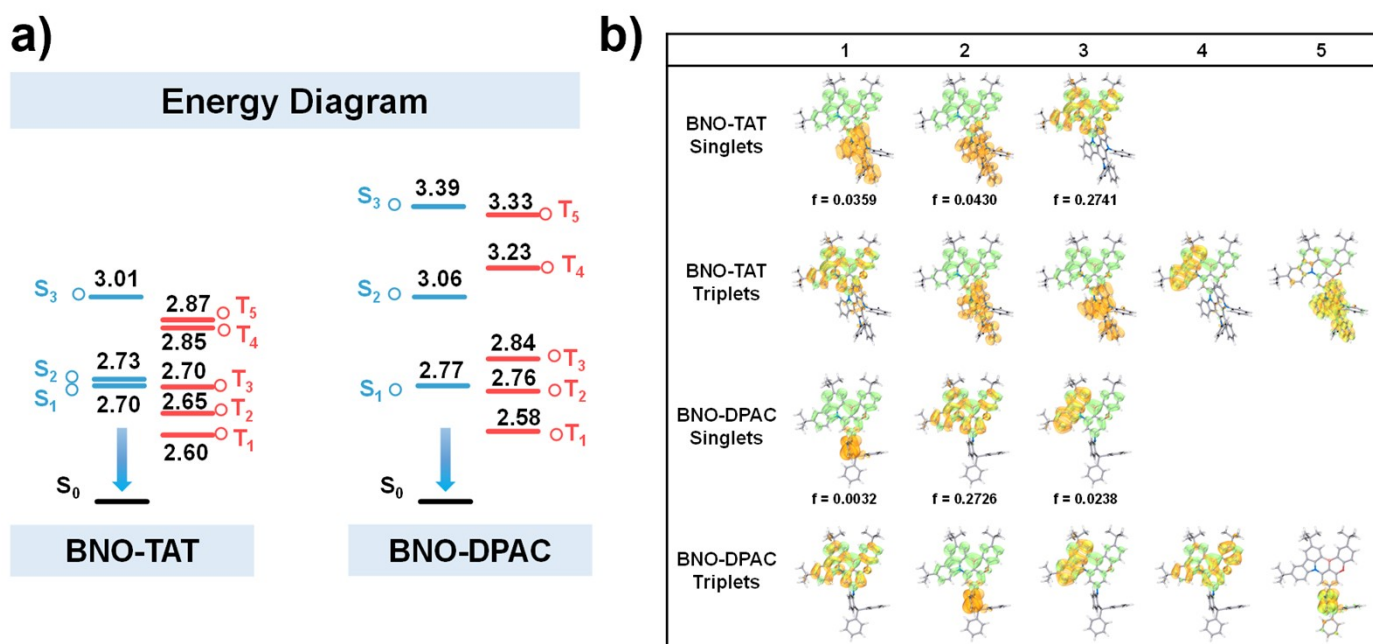


Fig. S11 a) The excited-state energy level and b) NTO distributions of **BNO-TAT** and **BNO-DPAC**

Photophysical Properties

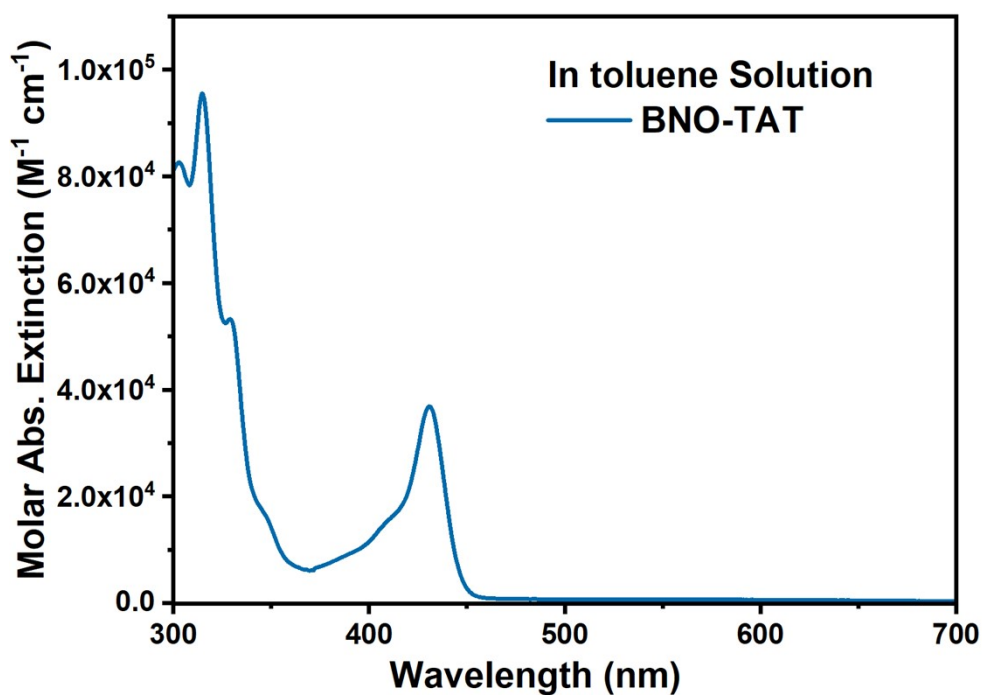


Fig. S12 UV-vis spectrum of **BNO-TAT** in toluene solution

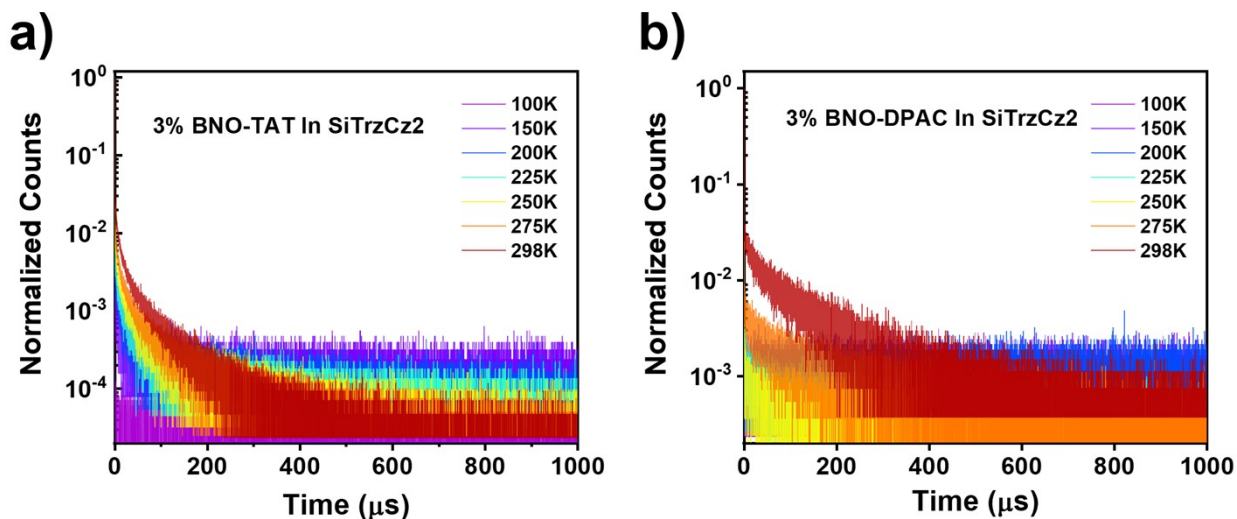


Fig. S13 Temperature-dependent transient PL decay curves of a) **BNO-TAT** and b) **BNO-DPAC**

Table S1 Photophysical data and kinetic parameters of 3 wt% emitters in SiTrzCz2 film

Emitter	λ_{em} [nm]	FWHM [nm]	PLQY [%]	τ_{PF} [ns]	τ_{DF} [μ s]	$R_{delayed}$ [%]	k_T [10^7 s $^{-1}$]	k_{ISC} [10^7 s $^{-1}$]	k_{RISC} [10^5 s $^{-1}$]
BNO-TAT	452	30	99%	10.0 \pm 0.3	28.4 \pm 0.2	68	3.2	6.8	1.1
BNO-DPAC	448	24	92%	6.1 \pm 0.2	66.2 \pm 0.2	52	7.2	8.5	0.3

Electroluminescence Devices

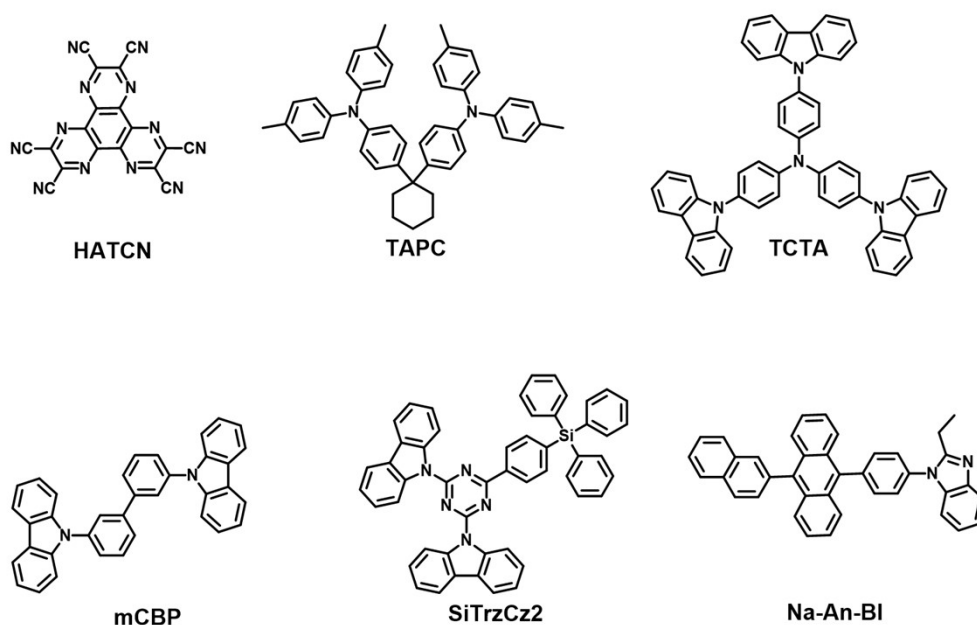


Fig. S14 Chemical structures of the materials used in the EL devices

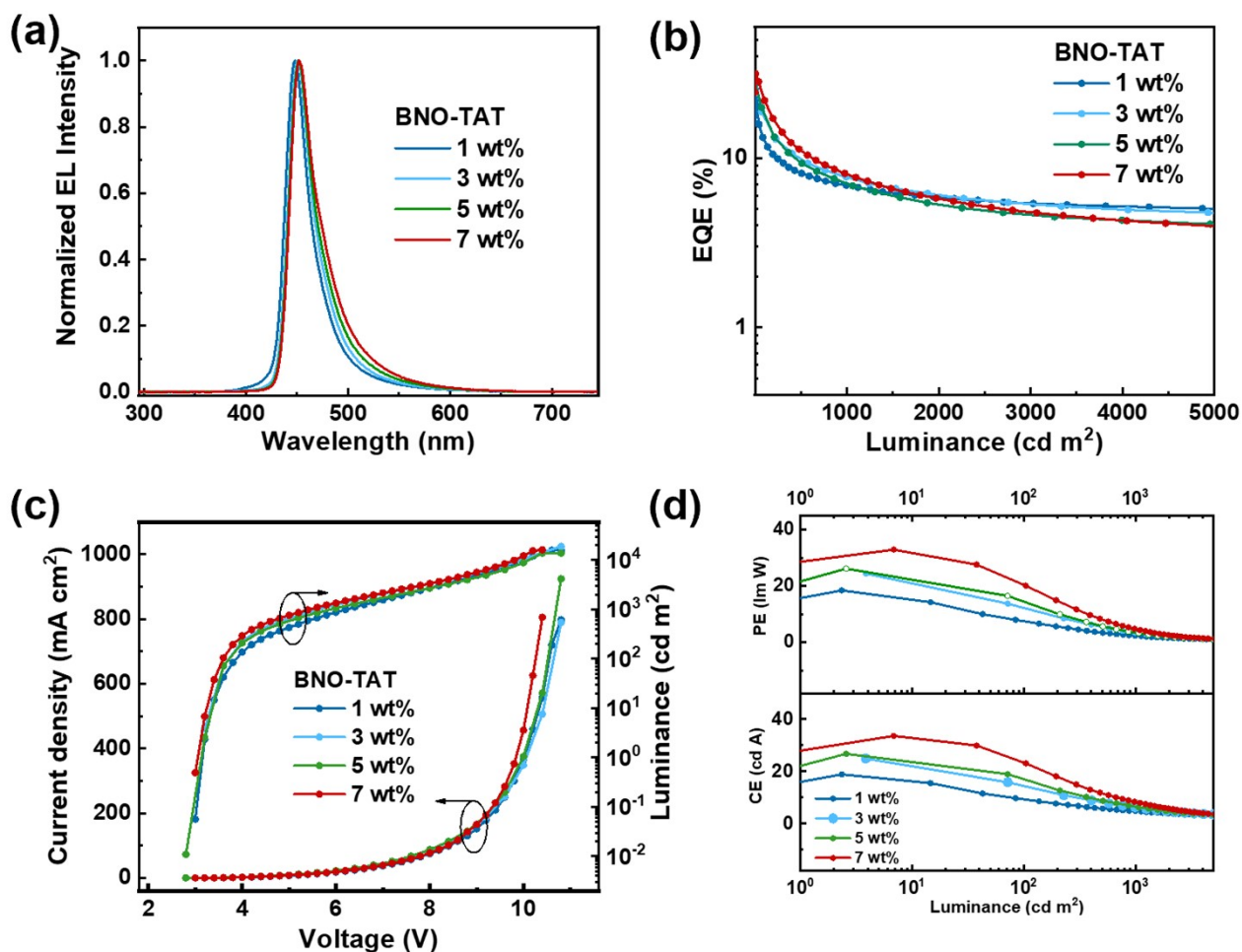


Fig. S15 EL devices: a) EL spectra b) EQE versus luminance curves; (c) current density and luminance versus voltage (J - V - L) characteristics; d) PE and CE versus brightness curves of the doped devices

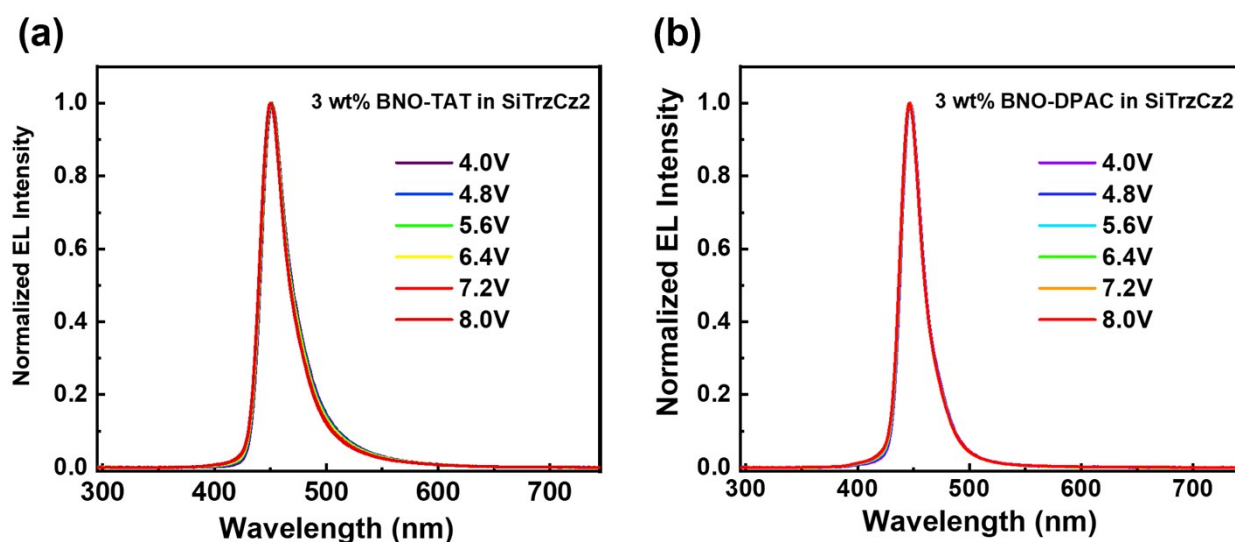


Fig. S16 EL spectra of the devices at various driving voltages.

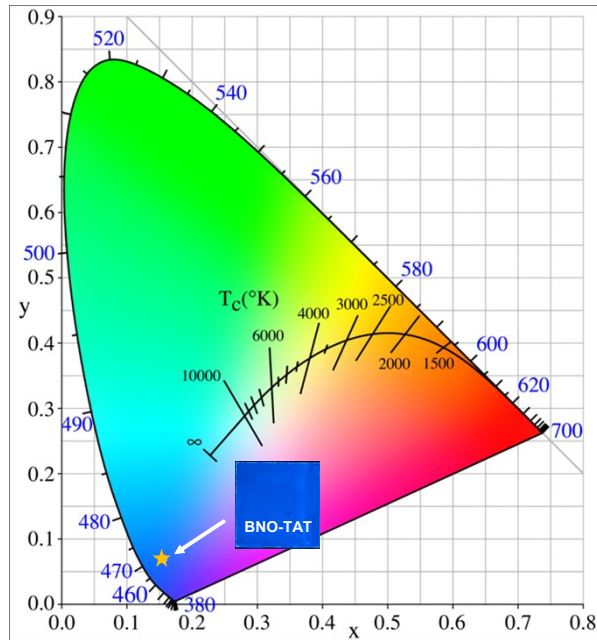


Fig. S17 Full-resolution CIE 1931 diagrams for the EL devices based on BNO-TAT

Table S2 Summary of EL devices performance

EML	$V_{on}^{[a]}$ (V)	$\lambda_{EL}^{[b]}$ (nm)	FWHM ^[b] (nm/eV)	CIE ^[b] (x, y)	$L_{max}^{[c]}$ (cd m ⁻²)	$PE_{max}^{[c]}$ (lm W ⁻¹)	$CE_{max}^{[c]}$ (cd A ⁻¹)	$EQE_{max/100/1000}^{[d]}$ (%)
1 wt% BNO-TAT	3.2	448	28	(0.156,0.069)	15780	18.5	18.9	25.8/12.2/6.8
3 wt% BNO-TAT	3.2	451	29	(0.151,0.083)	18916	24.5	25.0	29.5/17.5/7.5
5 wt% BNO-TAT	3.2	452	30	(0.151,0.098)	19085	26.3	26.7	27.8/18.6/7.6
7 wt% BNO-TAT	3.2	453	33	(0.151,0.114)	16074	33.0	33.6	31.6/22.3/7.7
3 wt% BNO-DPAC	3.2	446	23	(0.154,0.051)	10186	5.4	5.5	9.7/6.8/4.9

^[a] Turn-on voltage at 1 cd m⁻²; ^[b] electroluminescence peak wavelength, full-width at half-maximum, and CIE coordinates at 1000 cd m⁻²; ^[c] maximum luminance, maximum power efficiency, and maximum current efficiency; ^[d] external quantum efficiency at maximum, 100 cd m⁻² and 1000 cd m⁻².

References

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Cartesian Coordinates

Table S3 Cartesian coordinates of the model compound **BNO-TAT** at optimized S₀ geometry.

BNO-TAT at optimized S ₀ geometry			
C	-2.09258	0.741601	0.3273
C	-0.81375	1.301117	0.22516
C	0.304744	0.552721	0.613644
C	0.178655	-0.74882	1.090269
C	-1.09801	-1.30923	1.131544
C	-2.26144	-0.61071	0.753883
B	-3.61065	-1.34001	0.747336
O	-1.14633	-2.6	1.56641
N	-3.24853	1.447839	-0.02418
C	-2.32762	-3.27827	1.732415
C	-2.1877	-4.55419	2.290468
C	-3.31777	-5.31829	2.522701
C	-4.61292	-4.84209	2.220366
C	-4.70458	-3.57319	1.654441
C	-3.58296	-2.75386	1.374717
C	-5.83772	-5.72364	2.52508
C	-5.88251	-6.04038	4.038988
C	-7.16283	-5.03915	2.141031
C	-5.73052	-7.04604	1.728877
C	-4.47571	0.79881	-0.19494
C	-5.42392	1.703323	-0.71625
C	-4.76001	2.989304	-0.82222
C	-3.43033	2.811919	-0.36927

C	-5.21736	4.246631	-1.22431
C	-4.37433	5.359945	-1.16902
C	-3.06937	5.162565	-0.67292
C	-2.58476	3.920236	-0.26846
C	-4.76676	-0.53977	0.104778
C	-6.08047	-0.95039	-0.22218
C	-7.05109	-0.1	-0.77021
C	-6.70502	1.247266	-1.00052
C	-8.47425	-0.5783	-1.12202
C	-8.68475	-2.07486	-0.82426
C	-9.50706	0.224313	-0.29535
C	-8.73773	-0.35058	-2.62974
C	-4.81892	6.76788	-1.60646
C	-6.27316	6.788673	-2.11357
C	-4.71353	7.741041	-0.40825
C	-3.90332	7.263812	-2.75085
C	2.900013	-0.39611	-0.97542
C	4.213127	-0.84092	-1.28928
C	5.3663	-0.25024	-0.71471
C	5.170627	0.7385	0.28853
C	3.883114	1.217161	0.637407
C	2.762478	0.584461	0.03646
C	6.80427	-0.36002	-0.92433
C	7.415586	0.500181	0.021446
N	6.42198	1.164927	0.752885
C	3.362726	2.291597	1.474008
C	1.949627	2.200933	1.415509
N	1.589296	1.16361	0.541577
C	1.990898	-1.08634	-1.87962
C	2.78206	-1.98603	-2.63527
N	4.128536	-1.83357	-2.2746
C	7.637875	-1.04398	-1.8257
C	9.019482	-0.91274	-1.72459
C	9.599076	-0.10902	-0.73287
C	8.801346	0.610394	0.151557
C	3.923997	3.340586	2.221595
C	3.094905	4.206194	2.928904
C	1.702721	4.045953	2.914522
C	1.113134	3.039993	2.154171
C	0.61841	-1.00981	-2.17089
C	0.068777	-1.85554	-3.12938
C	0.863414	-2.78875	-3.81027
C	2.232715	-2.8622	-3.57323
C	6.708082	1.753875	2.019871
C	5.083938	-2.8582	-2.54099
C	5.477801	-3.11346	-3.85972
C	6.38086	-4.14274	-4.12839

C	6.901489	-4.91125	-3.08558
C	6.508662	-4.65213	-1.771
C	5.594491	-3.63634	-1.49631
C	7.509799	2.89938	2.087073
C	7.826635	3.454153	3.327642
C	7.33723	2.877702	4.501202
C	6.534976	1.737111	4.430438
C	6.227701	1.167539	3.195864
H	-0.64952	2.271937	-0.21301
H	1.041187	-1.32457	1.40087
H	-1.19571	-4.91703	2.537977
H	-3.19244	-6.3045	2.959593
H	-5.68224	-3.1686	1.430593
H	-6.74563	-6.67438	4.271218
H	-4.98442	-6.56876	4.372502
H	-5.96706	-5.12165	4.628396
H	-8.00157	-5.70226	2.376035
H	-7.21073	-4.8147	1.07046
H	-7.31482	-4.1067	2.694563
H	-5.70695	-6.85313	0.651449
H	-4.82643	-7.60562	1.986844
H	-6.59119	-7.69045	1.940699
H	-6.24036	4.3431	-1.56927
H	-2.39812	6.011391	-0.58892
H	-1.58667	3.860438	0.141147
H	-6.3392	-1.98642	-0.05171
H	-7.4382	1.935971	-1.41002
H	-9.70573	-2.36303	-1.0944
H	-8.00086	-2.70554	-1.40168
H	-8.54897	-2.30358	0.237781
H	-10.5257	-0.09806	-0.5391
H	-9.44325	1.298339	-0.49395
H	-9.35053	0.074276	0.777813
H	-8.02493	-0.9139	-3.24064
H	-9.7485	-0.68041	-2.89518
H	-8.65097	0.704638	-2.90521
H	-6.54268	7.804858	-2.41845
H	-6.41096	6.136535	-2.98227
H	-6.9805	6.479966	-1.33679
H	-5.02308	8.7489	-0.70702
H	-3.69093	7.808296	-0.02567
H	-5.3575	7.417938	0.416125
H	-2.85499	7.311757	-2.44213
H	-3.96519	6.598134	-3.61784
H	-4.20234	8.268323	-3.07094
H	7.223262	-1.66598	-2.6048
H	9.655112	-1.44473	-2.42605

H	10.6799	-0.03319	-0.65918
H	9.243036	1.243591	0.912053
H	4.992678	3.492306	2.251068
H	3.538369	5.014105	3.503074
H	1.072913	4.717347	3.490609
H	0.037108	2.913314	2.136237
H	-0.01716	-0.29334	-1.67108
H	-0.99254	-1.79002	-3.34891
H	0.41245	-3.45295	-4.54155
H	2.853847	-3.57146	-4.10763
H	5.088703	-2.49244	-4.65972
H	6.685549	-4.33499	-5.1528
H	7.610618	-5.70603	-3.29588
H	6.909824	-5.24646	-0.95564
H	5.278655	-3.43365	-0.47854
H	7.861894	3.355785	1.167935
H	8.446759	4.344374	3.374304
H	7.577699	3.315948	5.464979
H	6.151028	1.284168	5.339491
H	5.610796	0.277496	3.133262

Table S4 Cartesian coordinates of the model compound **BNO-DPAC** at optimized S₀ geometry.

BNO-DPAC at optimized S ₀ geometry			
C	0.914741	0.337578	0.111288
C	-0.46449	0.567726	0.046313
C	-1.35005	-0.51703	0.040982
C	-0.89247	-1.82876	0.085396
C	0.487702	-2.04272	0.105419
C	1.42817	-0.99504	0.104199
B	2.925039	-1.32595	0.017967
O	0.869991	-3.35142	0.108506
N	1.849338	1.379381	0.14149
C	2.185592	-3.73419	0.184079
C	2.380312	-5.11645	0.287307
C	3.668137	-5.61157	0.392174
C	4.794622	-4.75905	0.407066
C	4.555717	-3.39255	0.288215
C	3.262152	-2.82895	0.157488
C	6.203072	-5.36279	0.554411
C	6.476455	-6.32483	-0.62627
C	7.304477	-4.2864	0.560383
C	6.29187	-6.14784	1.884873
C	3.207608	1.146928	-0.09425
C	3.890925	2.377064	-0.19285
C	2.91078	3.419418	0.050555

C	1.668836	2.779338	0.279196
C	3.02299	4.809876	0.127802
C	1.913436	5.594653	0.454138
C	0.701367	4.926557	0.724513
C	0.558585	3.54246	0.650584
C	3.838519	-0.10019	-0.20866
C	5.220429	-0.04278	-0.50667
C	5.939922	1.152191	-0.64685
C	5.252273	2.370564	-0.46946
C	7.445336	1.183681	-0.97947
C	8.041132	-0.2261	-1.15363
C	7.666444	1.961089	-2.29899
C	8.211834	1.889306	0.164567
C	1.974153	7.130693	0.54555
C	3.374919	7.679272	0.214878
C	0.968233	7.745929	-0.45618
C	1.607985	7.580103	1.980065
C	-3.47633	0.101955	1.122192
C	-4.88743	0.127811	1.082944
C	-5.60547	-0.48066	-0.13453
C	-4.78297	-0.12973	-1.38586
C	-3.37507	-0.14272	-1.297
N	-2.76604	-0.28561	-0.03252
C	-2.80731	0.466359	2.303581
C	-3.52294	0.891843	3.418644
C	-4.91351	0.971415	3.373825
C	-5.57795	0.584932	2.210468
C	-5.3703	0.081047	-2.63806
C	-4.60371	0.241721	-3.79151
C	-3.21411	0.18825	-3.69666
C	-2.60156	0.004632	-2.46107
C	-7.03819	0.089378	-0.25719
C	-5.63221	-2.03539	0.029824
C	-8.18358	-0.71248	-0.23501
C	-9.45869	-0.14825	-0.35323
C	-9.61098	1.228015	-0.49588
C	-8.47452	2.041683	-0.52025
C	-7.20747	1.477911	-0.40272
C	-5.74726	-2.62638	1.296885
C	-5.81827	-4.01238	1.44327
C	-5.77366	-4.84346	0.32412
C	-5.66072	-4.27039	-0.94205
C	-5.59053	-2.8837	-1.08628
H	-0.87318	1.560823	-0.05098
H	-1.58439	-2.66204	0.087171
H	1.516756	-5.77311	0.292745
H	3.80204	-6.68589	0.47602

H	5.393454	-2.70911	0.318012
H	7.472927	-6.771	-0.53251
H	5.750064	-7.14218	-0.66371
H	6.430213	-5.79372	-1.58253
H	8.284355	-4.7627	0.666761
H	7.185753	-3.58699	1.394456
H	7.317664	-3.71111	-0.37112
H	6.110095	-5.48937	2.740429
H	5.561269	-6.96104	1.929083
H	7.287623	-6.59021	2.001442
H	3.988406	5.266033	-0.05844
H	-0.17114	5.503778	1.013781
H	-0.38976	3.100211	0.920666
H	5.742066	-0.97926	-0.64932
H	5.783795	3.313728	-0.55596
H	9.106802	-0.14761	-1.39146
H	7.951581	-0.82371	-0.24063
H	7.560807	-0.77364	-1.97117
H	8.733295	1.997912	-2.54667
H	7.306716	2.992066	-2.23129
H	7.14107	1.47887	-3.12968
H	7.868853	2.917616	0.312669
H	8.080633	1.354909	1.111073
H	9.283876	1.926472	-0.05958
H	3.368654	8.771716	0.283676
H	4.132981	7.310393	0.913634
H	3.686549	7.414754	-0.80093
H	0.994507	8.840019	-0.40018
H	-0.05792	7.42742	-0.25082
H	1.209096	7.452175	-1.48299
H	0.601121	7.260099	2.26364
H	2.308573	7.163967	2.711266
H	1.643471	8.672567	2.058287
H	-1.7265	0.422044	2.345888
H	-2.9841	1.170624	4.319641
H	-5.47839	1.311505	4.236042
H	-6.66138	0.614655	2.18118
H	-6.45197	0.096686	-2.71062
H	-5.08893	0.39264	-4.75066
H	-2.59692	0.302164	-4.58314
H	-1.52096	-0.01379	-2.39491
H	-8.08849	-1.78616	-0.12512
H	-10.3314	-0.79494	-0.33278
H	-10.6009	1.665538	-0.58754
H	-8.57573	3.117639	-0.63145
H	-6.33142	2.118725	-0.42355
H	-5.7758	-2.00111	2.181766

H	-5.90359	-4.44053	2.438202
H	-5.82341	-5.92259	0.437542
H	-5.6221	-4.90153	-1.82561
H	-5.49686	-2.46145	-2.08005

Table S5 Cartesian coordinates of the model compound **BNO-TAT** at the S_1 excited states.

BNO-TAT at the optimized S_1 geometry			
C	-1.93879	0.21558	0.850625
C	-0.55344	0.315088	1.045227
C	0.197445	-0.85282	1.189103
C	-0.3942	-2.12208	1.179035
C	-1.76453	-2.19659	0.934851
C	-2.5814	-1.06027	0.731212
B	-4.05766	-1.23944	0.352754
O	-2.27143	-3.46472	0.882665
N	-2.75633	1.348382	0.712063
C	-3.62515	-3.71681	0.694239
C	-3.97386	-5.0602	0.785442
C	-5.30536	-5.43874	0.616589
C	-6.30251	-4.47927	0.36724
C	-5.90492	-3.14159	0.279186
C	-4.56446	-2.70063	0.422524
C	-7.76765	-4.92986	0.206442
C	-8.23196	-5.65513	1.491726
C	-8.72532	-3.7497	-0.04398
C	-7.88114	-5.89983	-0.99347
C	-4.06558	1.252321	0.188676
C	-4.57937	2.539032	-0.03482
C	-3.57403	3.472681	0.412909
C	-2.47021	2.71242	0.893127
C	-3.55015	4.871711	0.479211
C	-2.46203	5.544204	1.037924
C	-1.40361	4.762724	1.554243
C	-1.39279	3.371417	1.496455
C	-4.77875	0.060754	-0.04518
C	-6.06582	0.263915	-0.61123
C	-6.61739	1.532201	-0.88082
C	-5.87123	2.678317	-0.57514
C	-8.0265	1.700195	-1.49012
C	-8.71346	0.353821	-1.78866
C	-8.92638	2.482908	-0.50467
C	-7.92746	2.48431	-2.82003
C	-2.3864	7.079911	1.130674
C	-3.6226	7.76521	0.518612
C	-2.28773	7.50947	2.613799

C	-1.13641	7.58428	0.371122
C	2.657498	-0.55502	-0.88114
C	3.914532	-0.28468	-1.54297
C	5.107336	-0.10265	-0.83865
C	5.083582	-0.3541	0.594689
C	3.879888	-0.53471	1.307271
C	2.667254	-0.62499	0.557055
C	6.482427	0.239446	-1.17735
C	7.239716	0.06624	0.003387
N	6.377111	-0.30627	1.058321
C	3.513196	-0.57303	2.715141
C	2.104051	-0.71789	2.733712
N	1.61757	-0.7482	1.434952
C	1.66607	-0.67864	-1.91094
C	2.342579	-0.48288	-3.15364
N	3.690131	-0.23645	-2.91968
C	7.144084	0.713212	-2.32003
C	8.521271	0.93517	-2.27556
C	9.25275	0.689503	-1.11138
C	8.61436	0.252622	0.053795
C	4.171637	-0.43968	3.948935
C	3.431332	-0.49603	5.125585
C	2.035952	-0.67406	5.112147
C	1.351073	-0.78037	3.912176
C	0.278386	-0.9671	-1.95343
C	-0.36199	-1.04577	-3.17393
C	0.339631	-0.85293	-4.38297
C	1.700162	-0.57655	-4.38865
C	6.888686	-0.81421	2.294851
C	4.64834	-0.33883	-3.97847
C	4.7338	0.686707	-4.92521
C	5.633433	0.571893	-5.98613
C	6.445824	-0.55858	-6.09721
C	6.350225	-1.58215	-5.15229
C	5.444259	-1.48131	-4.09678
C	7.614236	0.028923	3.142525
C	8.150189	-0.48251	4.324685
C	7.958868	-1.82479	4.659359
C	7.234837	-2.66011	3.806734
C	6.705344	-2.16139	2.617233
H	-0.0471	1.268097	1.029955
H	0.186082	-3.0263	1.320353
H	-3.20073	-5.79422	0.990443
H	-5.56026	-6.49184	0.688769
H	-6.65569	-2.38084	0.11345
H	-9.27161	-5.98971	1.392224
H	-7.61761	-6.53457	1.706288

H	-8.17049	-4.98786	2.357644
H	-9.75035	-4.121	-0.15124
H	-8.47143	-3.20722	-0.96012
H	-8.71565	-3.03647	0.786359
H	-7.56862	-5.4084	-1.92076
H	-7.25323	-6.78573	-0.85941
H	-8.91633	-6.23925	-1.11971
H	-4.40406	5.420608	0.098244
H	-0.56061	5.2539	2.03114
H	-0.57661	2.835585	1.962132
H	-6.64534	-0.61502	-0.85776
H	-6.27796	3.67013	-0.74671
H	-9.70399	0.532298	-2.22144
H	-8.1406	-0.2439	-2.50498
H	-8.8508	-0.24309	-0.88165
H	-9.93185	2.618033	-0.92179
H	-8.51924	3.473959	-0.28436
H	-9.02071	1.94515	0.444432
H	-7.30232	1.947243	-3.54119
H	-8.92108	2.619441	-3.26457
H	-7.48836	3.475524	-2.67493
H	-3.52176	8.852885	0.598894
H	-3.73884	7.519895	-0.54204
H	-4.54352	7.479411	1.036884
H	-2.22644	8.601242	2.696191
H	-1.40314	7.088512	3.100813
H	-3.16628	7.17427	3.17452
H	-0.21462	7.162157	0.78241
H	-1.18608	7.306326	-0.68689
H	-1.06104	8.676505	0.4336
H	6.604466	0.923322	-3.23063
H	9.025989	1.303965	-3.1623
H	10.32562	0.852185	-1.09974
H	9.173907	0.075851	0.964109
H	5.236651	-0.2786	4.007412
H	3.946573	-0.39418	6.075732
H	1.48871	-0.71529	6.048218
H	0.275506	-0.89688	3.869733
H	-0.27767	-1.13917	-1.04971
H	-1.42365	-1.26258	-3.19809
H	-0.19137	-0.92599	-5.32678
H	2.244472	-0.44164	-5.31516
H	4.106909	1.565897	-4.81742
H	5.701817	1.367986	-6.72082
H	7.14808	-0.64358	-6.92053
H	6.9752	-2.4652	-5.24036
H	5.353221	-2.27684	-3.36462

H	7.734617	1.075795	2.884554
H	8.708127	0.171388	4.987366
H	8.371929	-2.21805	5.582766
H	7.084203	-3.70362	4.06378
H	6.147195	-2.80409	1.944899

Table S6 Cartesian coordinates of the model compound **BNO-DPAC** at the S_1 excited states.

BNO-DPAC at the optimized S_1 geometry			
C	-0.9325	0.326269	-0.15016
C	0.450904	0.548976	-0.08439
C	1.30923	-0.55198	-0.08603
C	0.844929	-1.86925	-0.14006
C	-0.53571	-2.06161	-0.15144
C	-1.47154	-1.00222	-0.13228
B	-2.97008	-1.31137	-0.03456
O	-0.92898	-3.36843	-0.15848
N	-1.85439	1.382682	-0.18143
C	-2.26679	-3.74185	-0.22359
C	-2.47181	-5.11237	-0.34159
C	-3.77258	-5.6082	-0.41976
C	-4.87913	-4.74124	-0.39311
C	-4.62436	-3.37188	-0.2686
C	-3.32534	-2.81305	-0.16477
C	-6.30247	-5.3222	-0.50177
C	-6.55808	-6.28666	0.680664
C	-7.39007	-4.23202	-0.47009
C	-6.44564	-6.09954	-1.83177
C	-3.22679	1.169803	0.086019
C	-3.88247	2.405361	0.194909
C	-2.89499	3.426051	-0.0627
C	-1.65828	2.768326	-0.31748
C	-2.98046	4.822124	-0.13369
C	-1.86853	5.592418	-0.47888
C	-0.66755	4.910681	-0.77812
C	-0.54749	3.524827	-0.70868
C	-3.86453	-0.08002	0.196946
C	-5.24743	0.006876	0.508012
C	-5.94804	1.220624	0.654598
C	-5.25967	2.428763	0.481231
C	-7.45512	1.261921	0.988931
C	-8.06652	-0.141	1.166861
C	-7.67298	2.042662	2.306657
C	-8.21937	1.970663	-0.15438
C	-1.91056	7.129807	-0.56455

C	-3.29545	7.698385	-0.20227
C	-0.87608	7.731961	0.415788
C	-1.57021	7.582191	-2.0045
C	3.483098	-0.14991	-1.16675
C	4.904819	-0.06477	-1.12256
C	5.650316	-0.48141	0.148769
C	4.770853	-0.1711	1.360294
C	3.354138	-0.22715	1.243525
N	2.75448	-0.33481	-0.00363
C	2.795307	0.01473	-2.39693
C	3.496653	0.32696	-3.5453
C	4.887348	0.485514	-3.49409
C	5.573223	0.282433	-2.29324
C	5.316784	0.037273	2.623121
C	4.50755	0.164723	3.756041
C	3.115891	0.064681	3.639645
C	2.538043	-0.1317	2.399314
C	6.99926	0.263345	0.277858
C	5.843566	-2.03935	0.053272
C	8.212336	-0.39843	0.491647
C	9.400825	0.323057	0.646009
C	9.393785	1.714369	0.590494
C	8.186175	2.3866	0.384212
C	7.003379	1.668024	0.233377
C	6.384957	-2.60736	-1.11168
C	6.593833	-3.98064	-1.21374
C	6.253741	-4.82578	-0.15624
C	5.712669	-4.27768	1.00336
C	5.510915	-2.89898	1.108631
H	0.857999	1.543837	0.015959
H	1.516226	-2.71981	-0.15066
H	-1.61278	-5.77532	-0.37336
H	-3.91612	-6.68082	-0.50898
H	-5.45672	-2.68122	-0.27013
H	-7.56447	-6.7176	0.616886
H	-5.84128	-7.11321	0.69232
H	-6.47333	-5.75993	1.636844
H	-8.37988	-4.69444	-0.54959
H	-7.2843	-3.52912	-1.30262
H	-7.36543	-3.65985	0.46267
H	-6.27831	-5.43818	-2.68823
H	-5.72684	-6.92139	-1.90152
H	-7.4515	-6.5268	-1.92256
H	-3.93556	5.291268	0.073968
H	0.205161	5.478011	-1.0877
H	0.386784	3.067572	-1.00582
H	-5.78395	-0.92044	0.653407

H	-5.77535	3.380458	0.563786
H	-9.132	-0.05186	1.405419
H	-7.98027	-0.74144	0.25581
H	-7.58838	-0.69153	1.983427
H	-8.73978	2.08793	2.557263
H	-7.30236	3.069349	2.236201
H	-7.14883	1.557182	3.136531
H	-7.86604	2.99502	-0.30402
H	-8.0886	1.433516	-1.09953
H	-9.29266	2.015045	0.067094
H	-3.27634	8.791436	-0.26779
H	-4.07286	7.340003	-0.8846
H	-3.58893	7.432334	0.818339
H	-0.88646	8.827112	0.363054
H	0.140557	7.396973	0.189004
H	-1.10048	7.438723	1.446608
H	-0.57531	7.246326	-2.31183
H	-2.29319	7.177585	-2.72019
H	-1.59099	8.675855	-2.0801
H	1.719241	-0.07842	-2.41122
H	2.962413	0.465775	-4.47849
H	5.439667	0.75821	-4.38721
H	6.650752	0.394279	-2.26956
H	6.394092	0.086453	2.727086
H	4.964777	0.330709	4.725805
H	2.484002	0.150222	4.516586
H	1.464886	-0.19132	2.290936
H	8.238428	-1.4805	0.54015
H	10.33122	-0.21217	0.81014
H	10.31729	2.2728	0.708399
H	8.164657	3.471429	0.342969
H	6.070781	2.203202	0.079568
H	6.650254	-1.97756	-1.95238
H	7.016466	-4.38972	-2.12641
H	6.40625	-5.89727	-0.23881
H	5.440024	-4.91881	1.83597
H	5.092822	-2.50722	2.026973
