Supporting Information

Investigating the Effects of Planarized Versus Twisted Donors on a Multiple Resonance Thermally Activated Delayed Fluorescence Core

Mitchell J. Demchuk, Ryoga Hojo, Changfeng Si, Zachary M. Hudson

Department of Chemistry, The University of British Columbia, 2036 Main Mall, Vancouver, British Columbia, Canada, V6T 1Z1.

Tel: +1-604-822-3266; Fax: +1-604-822-2847; e-mail: zhudson@chem.ubc.ca.

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NMR Spectra

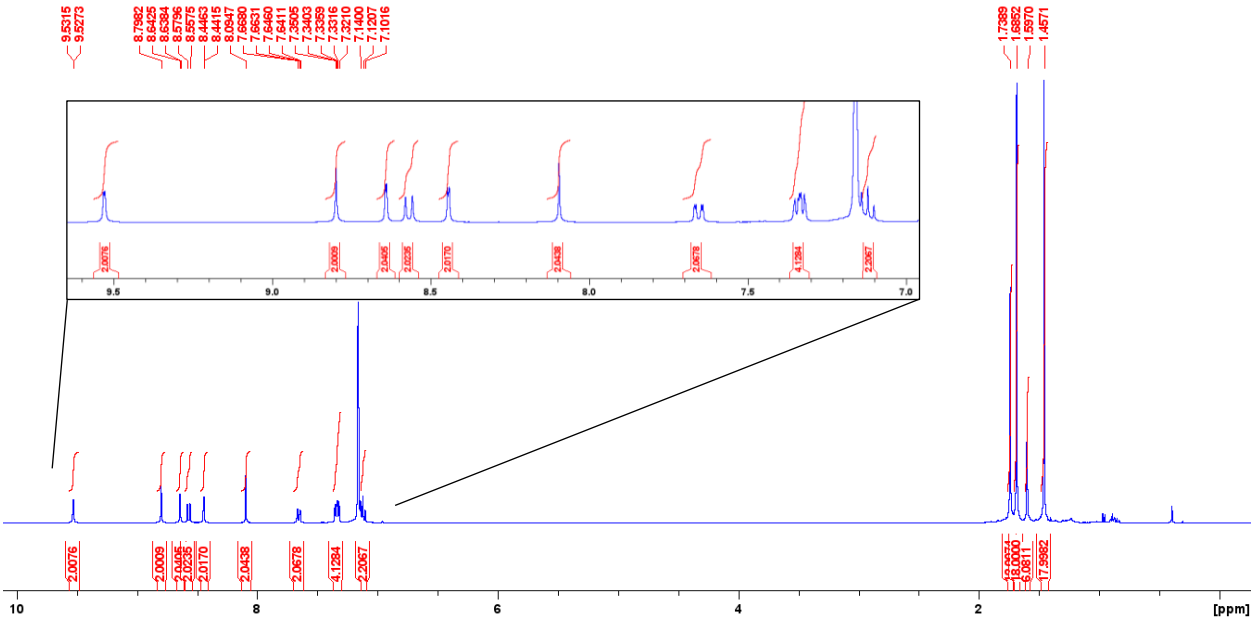

Figure S1. HMAT-BNCz: ^{1}H NMR, C_6D_6, 400 MHz, 298 K.

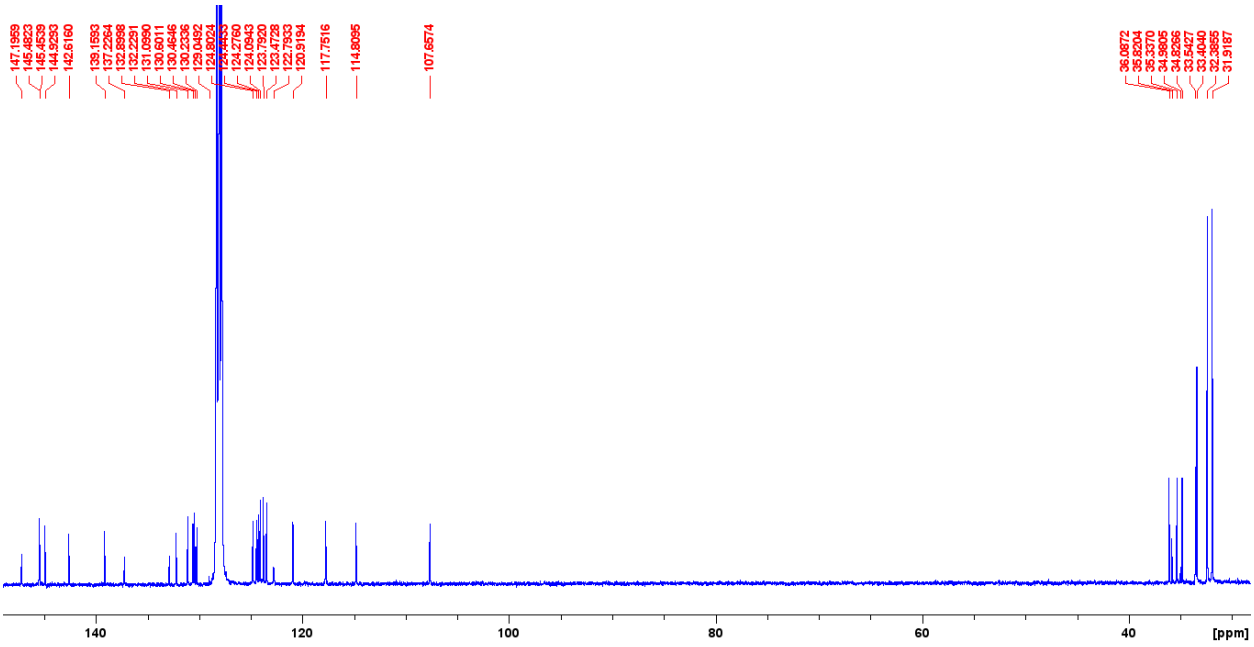

Figure S2. HMAT-BNCz: ^{13}C NMR, C_6D_6, 101 MHz, 298 K (Enhanced zoom).

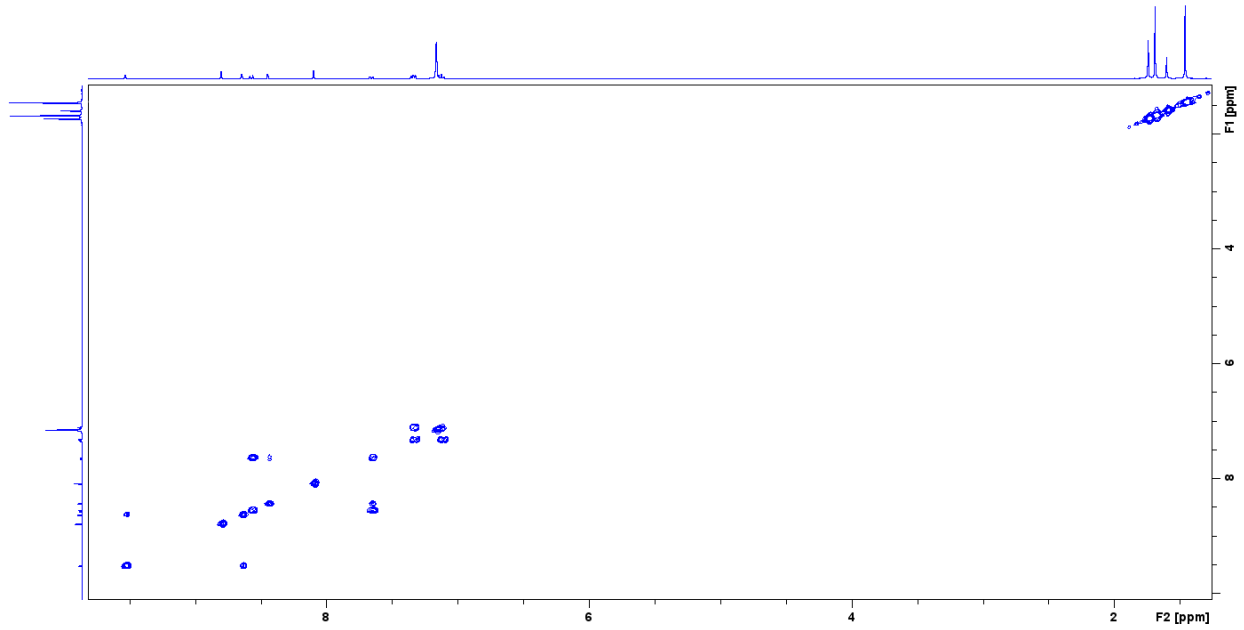

Figure S3. HMAT-BNCz: ^{1}H-^{1}H COSY 2D NMR, C_6D_6, 400 MHz, 298 K.

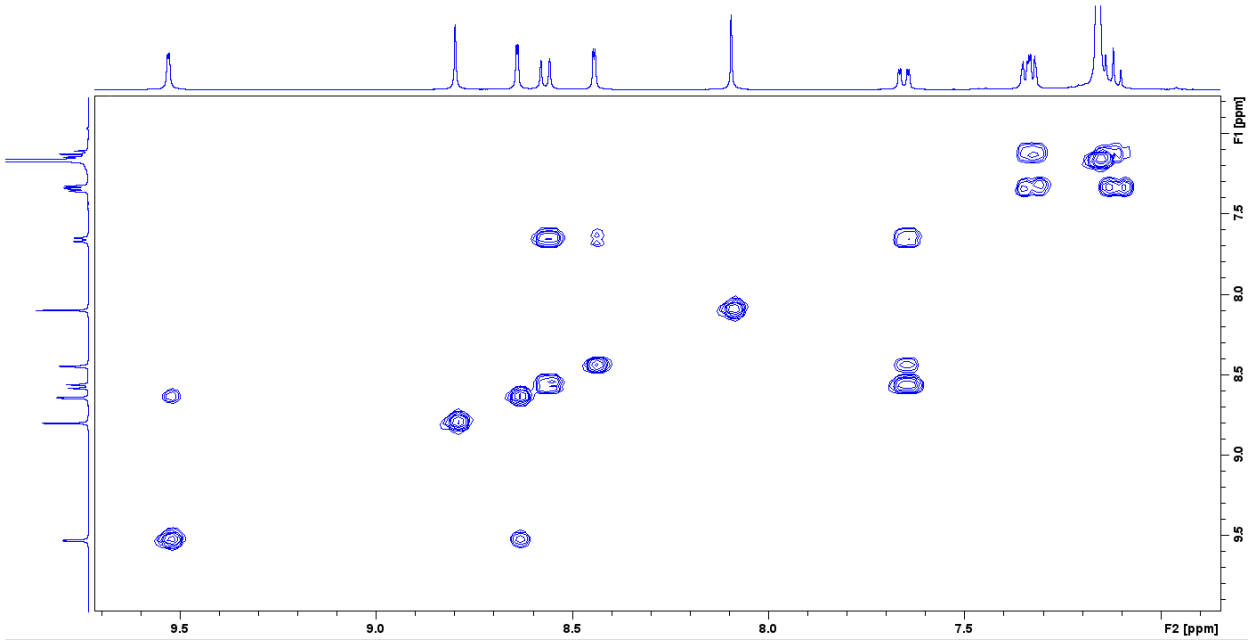

Figure S4. HMAT-BNCz: ^{1}H-^{1}H COSY 2D NMR, C_6D_6, 400 MHz, 298 K (Enhanced zoom).

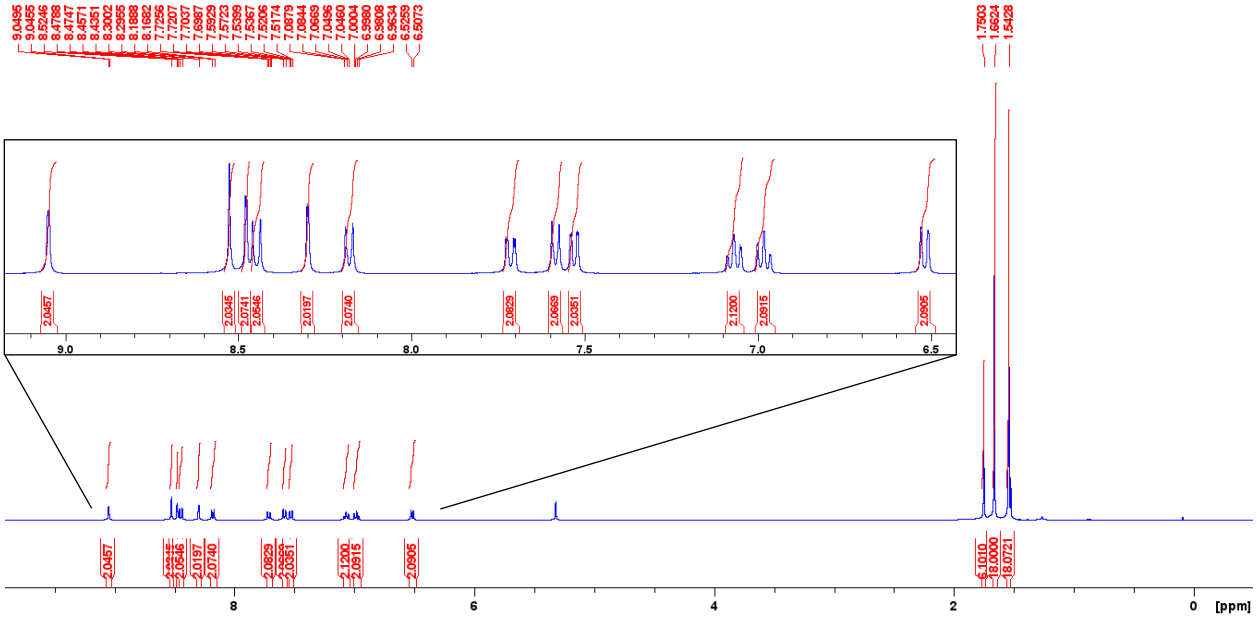

Figure S5. ACR-BNCz: ^{1}H NMR, CD_2Cl_2, 400 MHz, 298 K.

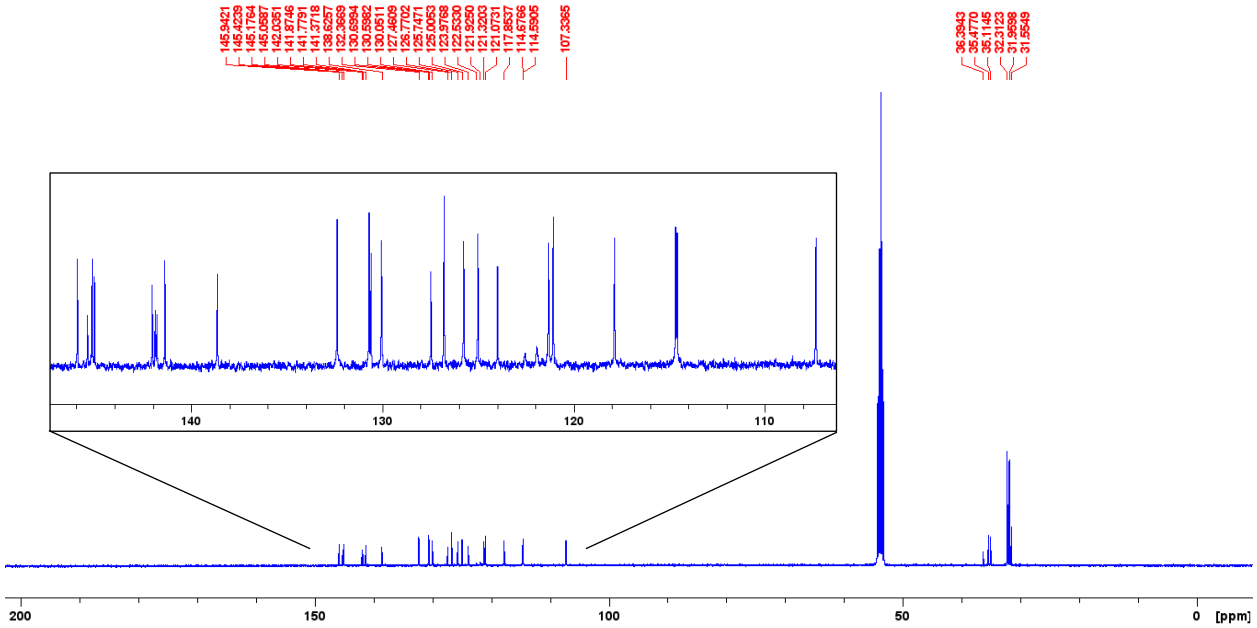

Figure S6. ACR-BNCz: ^{13}C NMR, CD_2Cl_2, 101 MHz, 298 K.

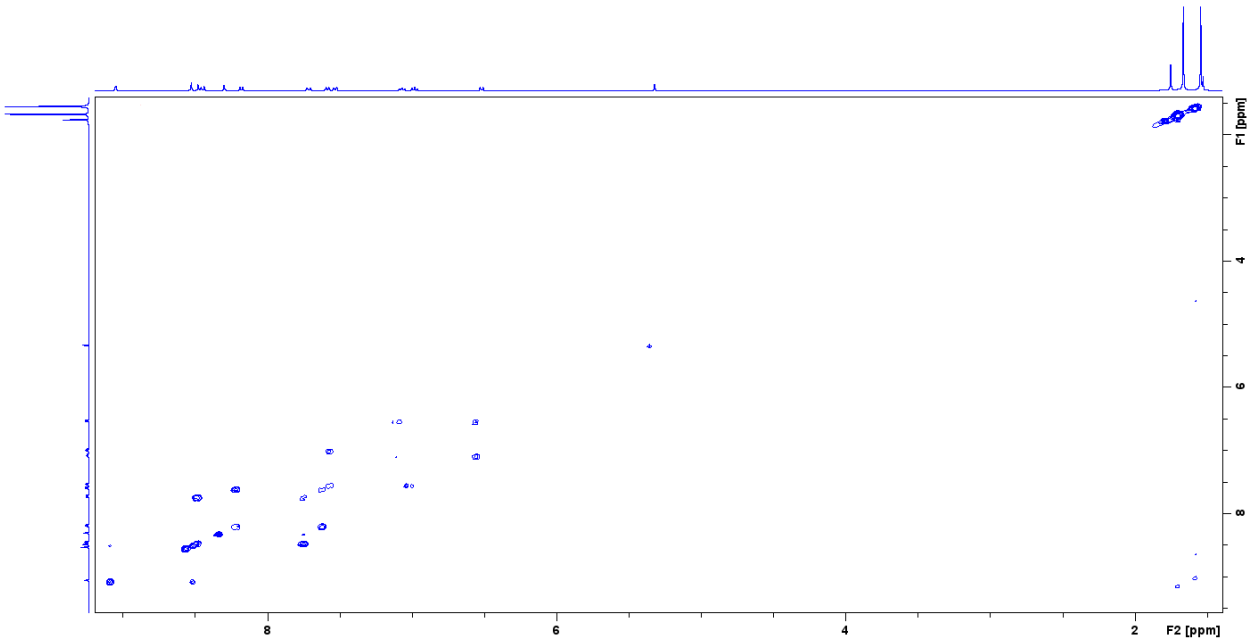

Figure S7. HMAT-BNCz: ^{1}H-^{1}H COSY 2D NMR, CD_2Cl_2, 400 MHz, 298 K.

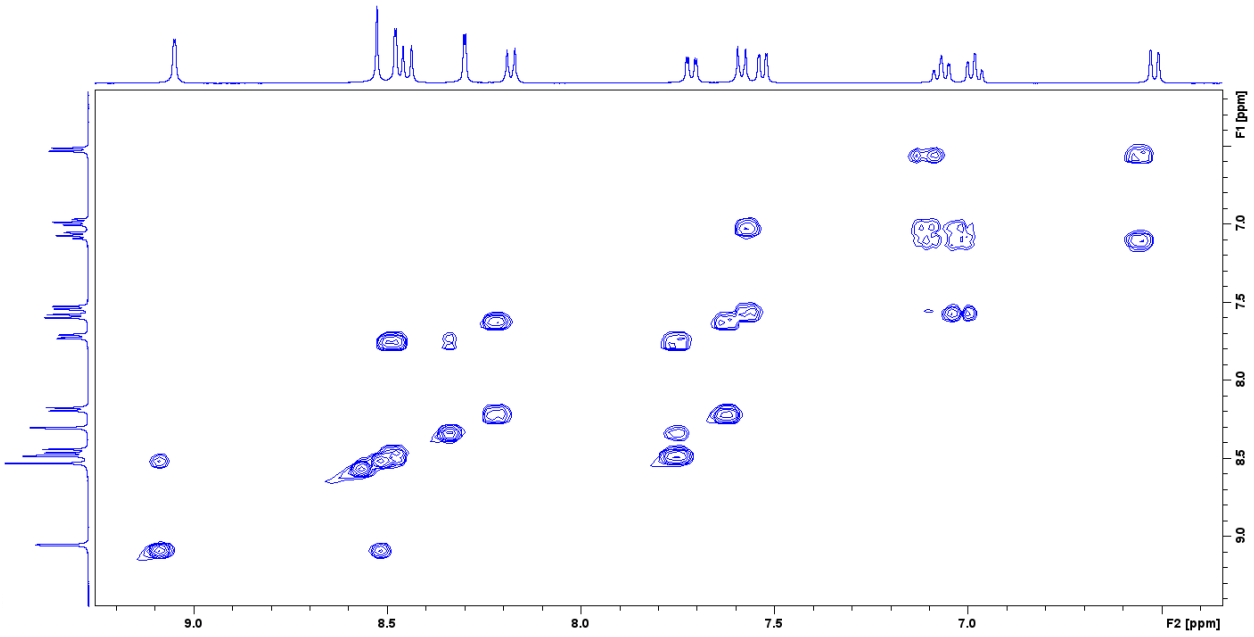

Figure S8. HMAT-BNCz: ^{1}H-^{1}H COSY 2D NMR, CD_2Cl_2, 400 MHz, 298 K (Enhanced zoom).

Photophysical and Electrochemical Characterization

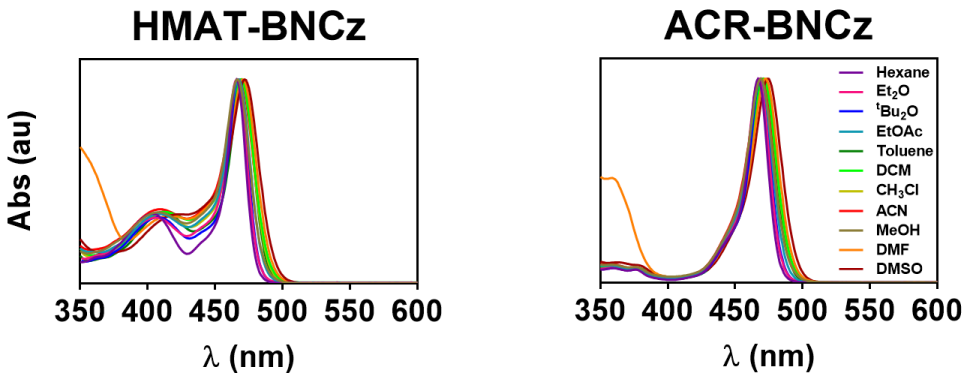

Figure S9. UV-Vis absorbance plots (normalized) of solvatochromism experiments used in Lippert-Mataga analysis. Spectra collected using 10 μM solutions of **HMAT-BNCz** or **ACR-BNCz** in each solvent.

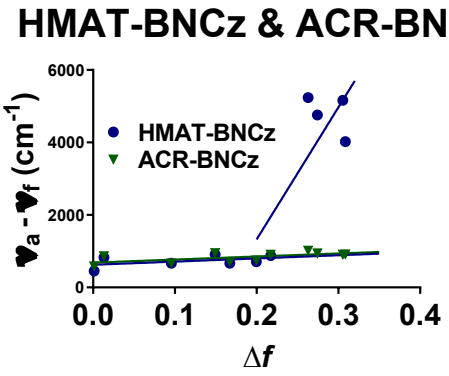

Figure S10. Lippert-Mataga plot combing results for both **HMAT-BNCz** and **ACR-BNCz**.

The Lippert-Mataga equation describes the relationship between a solute's dipole moment and the solvent it is interacting with. This equation is used to gain insight into how various solvents affect the optical properties of a solute:

$$(v_a - v_f) = \frac{2(u_e - u_g)^2}{hca^3}\Delta f + (v_a^0 - v_f^0)$$

Equation S1. Lippert-Mataga relationship

One can solve this equation to find the excited state dipole moment u_e, by applying the principle that **Equation S1** can be related to the expression $y = mx + b$. Plotting $(v_a - v_f)$ on the y-axis and Δf on the x-axis, we see a linear trend between these two variables which can be analyzed by

linear regression analysis to obtain a slope with units of cm^{-1}. By rearranging **Equation S1** we can solve for u_e by finding the experimental $(u_e - u_g)$ value.

$$\sqrt{\frac{mhca^3}{2}} = (u_e - u_g)$$

Equation S2. Rearranged Lippert-Mataga relationship

where $(v_a - v_f)$ is the Stokes shift, u_e is the excited state dipole moment, u_g is the ground state dipole moment, a is the Onsager cavity radius, Δf is the orientational polarizability of the solvent, and $(v_a^0 - v_f^0)$ is the Stokes shift when Δf is zero and m is slope of the Lippert-Mataga plot. The Onsager cavity radius (a) and Δf are defined by the equations:

$$a = (\frac{3M}{4N\pi d})^{\frac{1}{3}}$$

Equation S3. Onsager cavity radius

Where M is molecular weight of the solute, N is Avogadro's number, and d is the density of the molecule (assumed to be 1.0 g/cm^3).

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}$$

Equation S4. Orientational polarizability of a solvent

Where ε is the solvent dielectric constant, and n is the solvent refractive index.

The ground state dipole moments were calculated using density functional theory (DFT) calculations at the TPSSH/def2SVP level of theory. **HMAT-BNCz** has a u_g of 1.5 Debye and **ACR-BNCz** has a u_g of 1.4 Debye.

Table S1. Solvent constants and compound absorption and emission peaks in nm, along with stokes shift values in cm^{-1}.

Solvent	ε	n	Δf	HMAT-BNCz			ACR-BNCz		
				λ_a (nm)	λ_f (nm)	$\nu_a - \nu_f$ (cm^{-1})	λ_a (nm)	λ_f (nm)	$\nu_a - \nu_f$ (cm^{-1})
Hexane	1.90	1.375	0.0013	466	476	451	466	479	582
Toluene	2.38	1.497	0.0132	470	489	827	471	491	865
Di-tertbutyl ether	3.08	1.399	0.0957	467	482	666	469	484	661
Diethyl ether	4.34	1.352	0.1672	466	481	669	468	484	706
Chloroform	4.81	1.443	0.1492	469	490	914	471	493	947
Ethyl Acetate	6.02	1.372	0.1996	467	483	709	469	486	746
Dichloromethane	8.93	1.424	0.2171	468	488	876	470	491	910
Methanol	32.70	1.328	0.3086	467	575	4022	469	490	914
Dimethylformamide	36.70	1.431	0.2744	471	607	4757	472	494	944
Acetonitrile	37.50	1.344	0.3054	468	617	5160	470	491	910

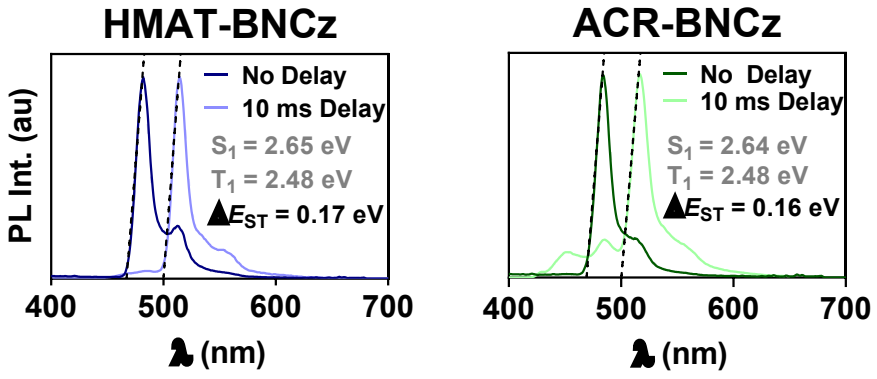

Figure S11. Phosphorimetry experimental spectra conducted in a 10 μM 2-MeTHF glass at 77 K using 375 nm excitation for **HMAT-BNCz** and **ACR-BNCz**. Initial spectra were taken as a steady state measurement, while the next spectra were taken with a 10 ms delay.

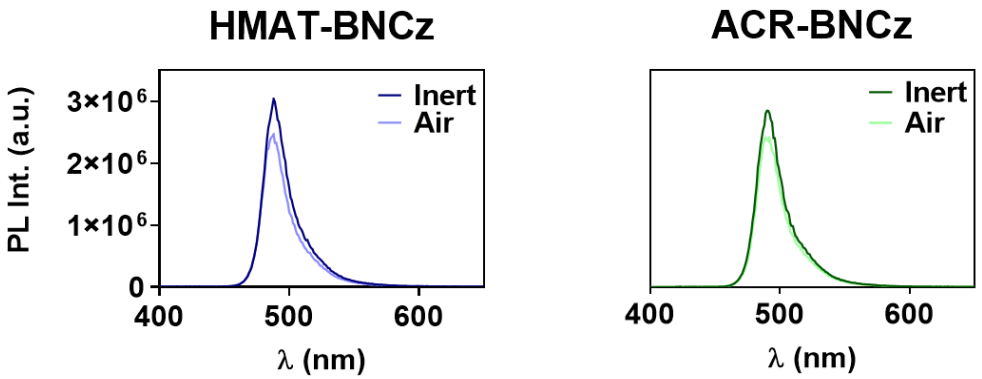

Figure S12. PL emission spectra for toluene solutions at 10 μM under air or nitrogen, 375 nm excitation.

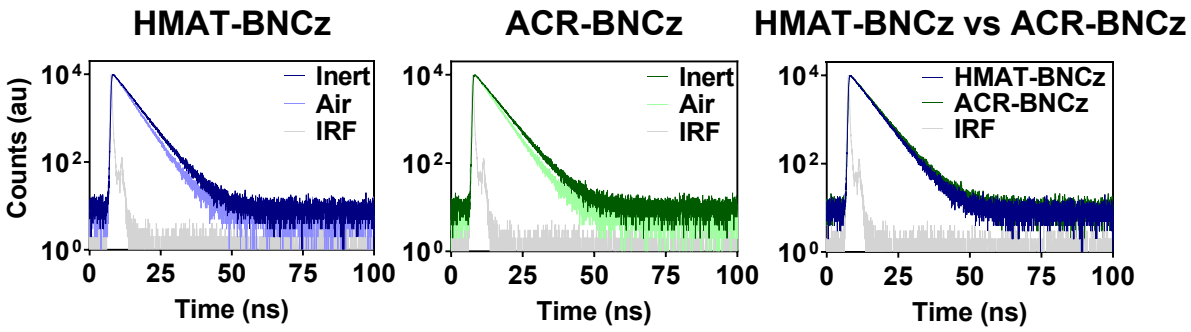

Figure S13. PL decays for toluene solutions at 10 μM under air or nitrogen. All measurements were performed using TCSPC with a 375 nm EPLED source.

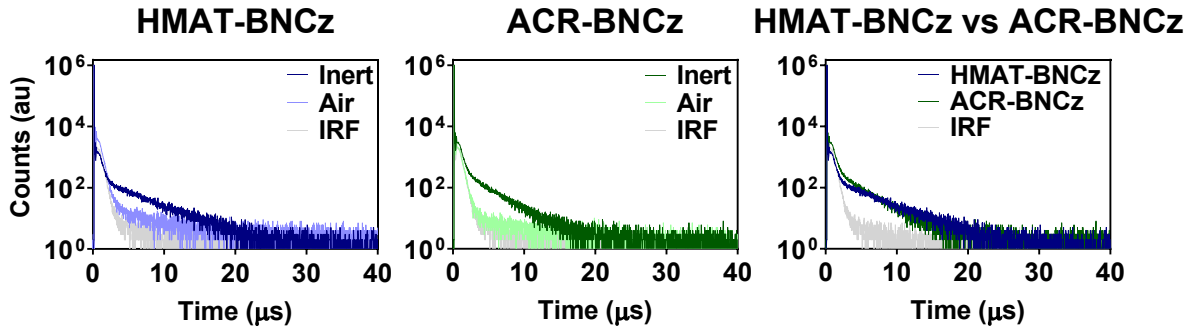

Figure S14. PL decays for toluene solutions at 10 μM under air or nitrogen. All measurements were performed using MCS with a 375 nm EPLED source.

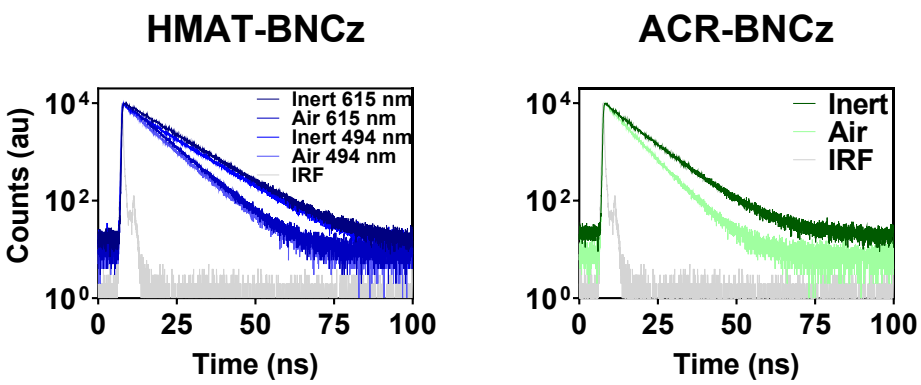

Figure S15. PL decays for acetonitrile solutions at 10 µM under air or nitrogen. All measurements were performed using TCSPC with a 375 nm EPLED source. HMAT-BNCz lifetimes probed at emission wavelengths of both 615 nm and 494 nm.

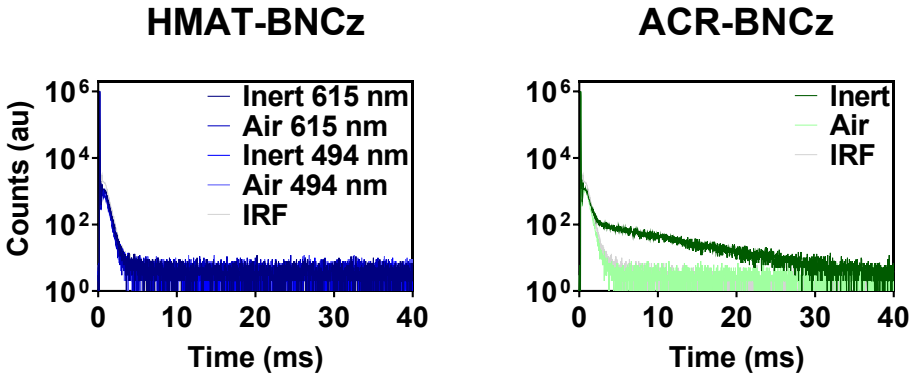

Figure S16. PL decays for acetonitrile solutions at 10 µM under air or nitrogen. All measurements were performed using MCS with a 375 nm EPLED source. HMAT-BNCz lifetimes probed at emission wavelengths of both 615 nm and 494 nm.

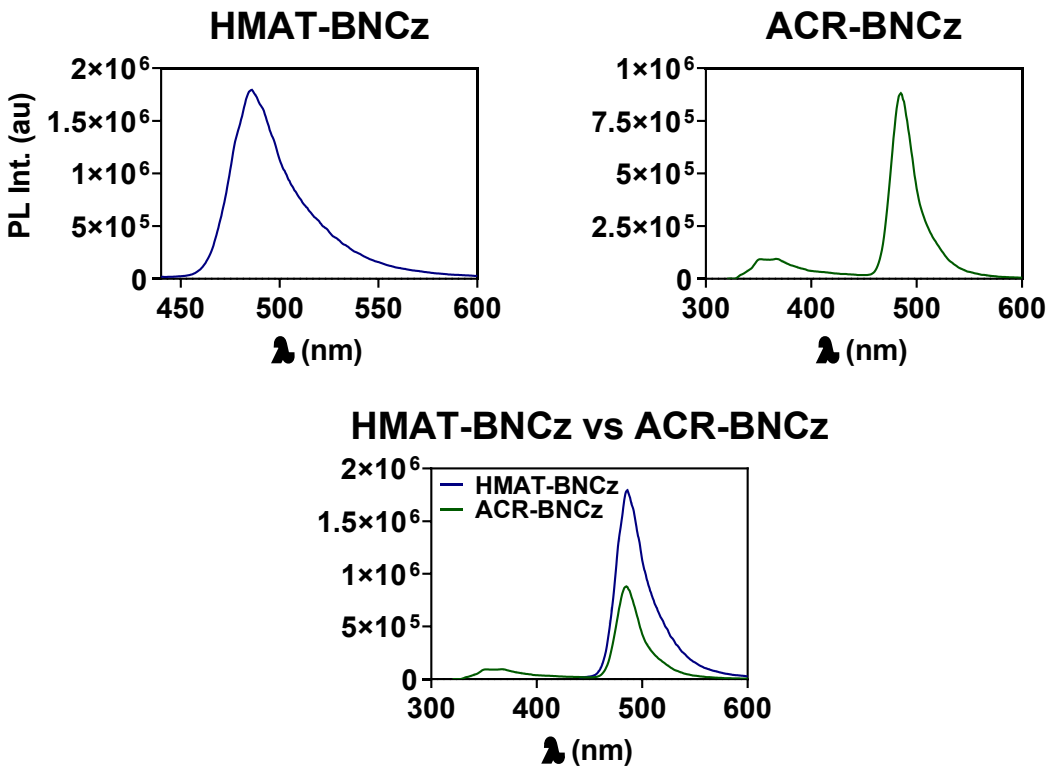

Figure S17. Emission spectra measured in 1 wt.% doped PMMA films under Ar. 300 nm excitation was used for **HMAT-BNCz**, while 375 nm was used for **ACR-BNCz**.

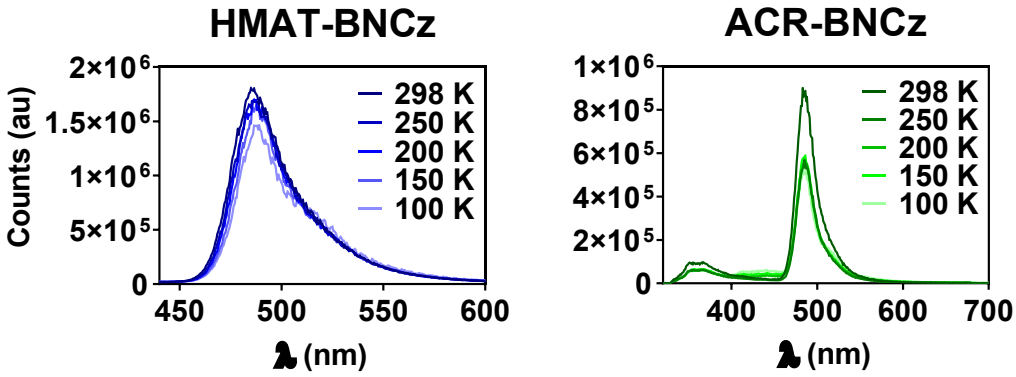

Figure S18. Steady-state emission spectra measured in 1 wt.% doped PMMA films under Ar from 298 K to 100 K. 300 nm excitation was used for **HMAT-BNCz**, while 375 nm was used for **ACR-BNCz**.

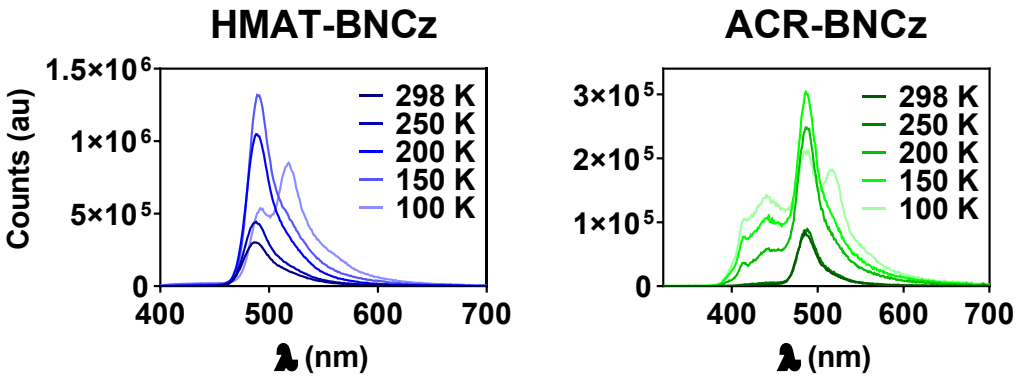

Figure S19. Time-Gated emission spectra measured in 1 wt.% doped PMMA films under Ar from 298 K to 100 K. 300 nm excitation was used for **HMAT-BNCz**, while 375 nm was used for **ACR-BNCz**. Gating was performed with a 200 μs window.

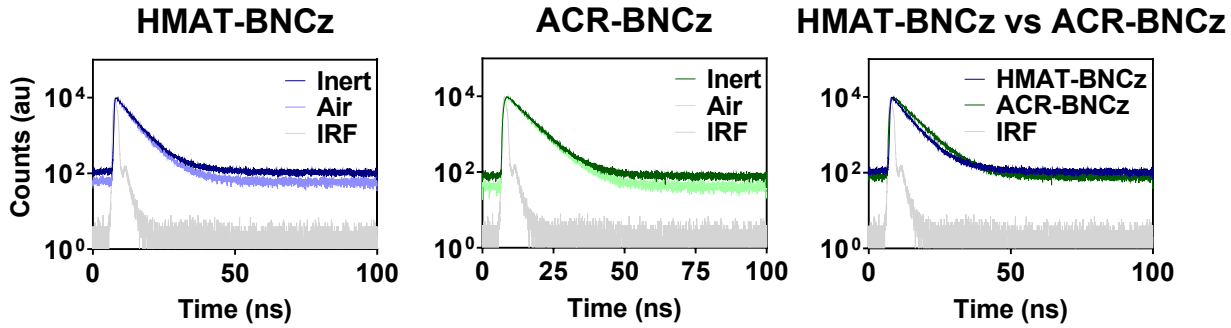

Figure S20. PL decays for 1 wt.% doped PMMA films under air or Ar. All measurements were performed using a TCSPC EPLED source with 300 nm excitation for **HMAT-BNCz** and 375 nm for **ACR-BNCz**.

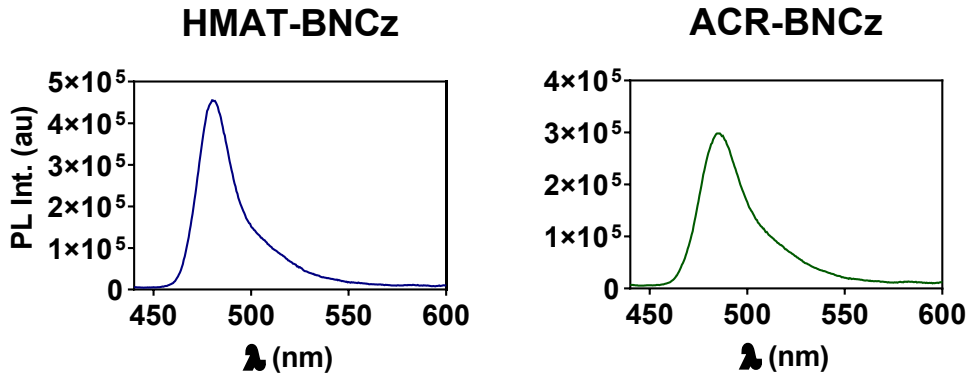

Figure S21. Emission spectra measured in 1 wt.% doped Zeonex films under Ar, 375 nm excitation.

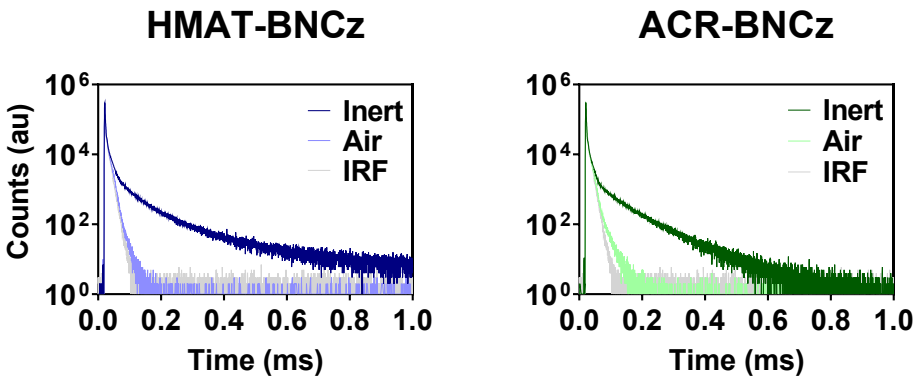

Figure S22. PL decays for 1 wt.% doped Zeonex films under air or Ar. Measurements were performed using a xenon μF lamp with MCS under 375 nm excitation.

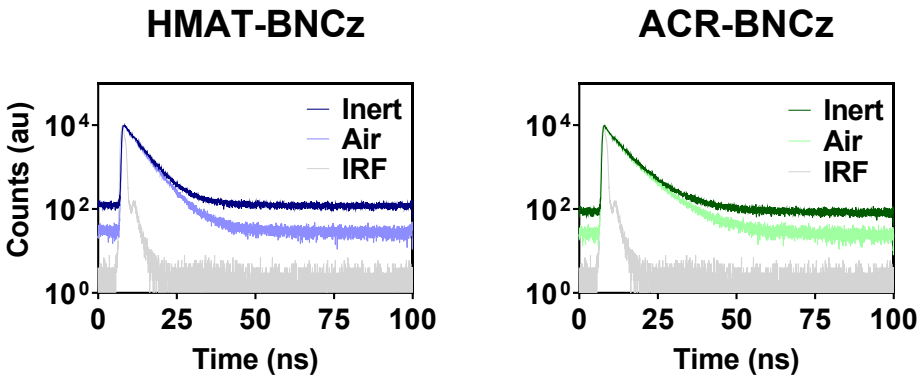

Figure S23. PL decays for 1 wt.% doped Zeonex films under air or Ar. All measurements were performed using a TCSPC EPLED source with 375 nm excitation.

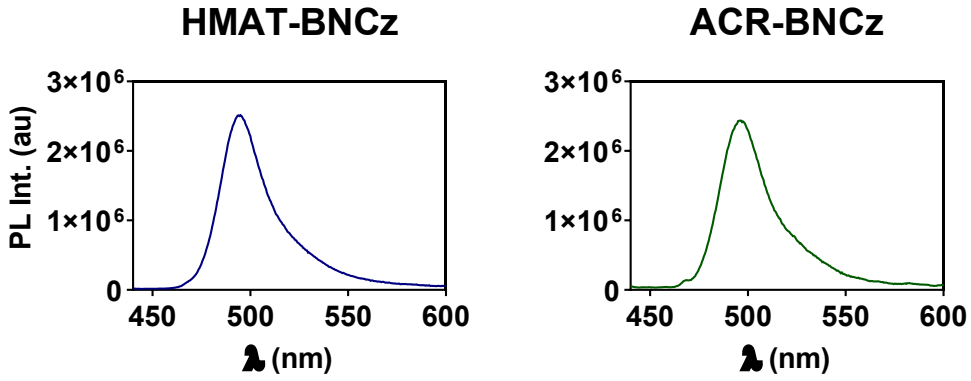

Figure S24. Emission spectra measured in 1 wt.% doped mCP films under Ar, 375 nm excitation.

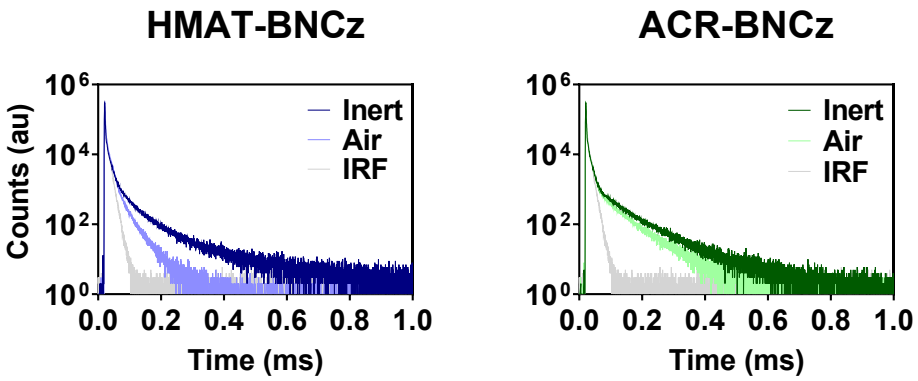

Figure S25. PL decays for 1 wt.% doped mCP films under air or Ar. Measurements were performed using a xenon μF lamp with MCS under 375 nm excitation.

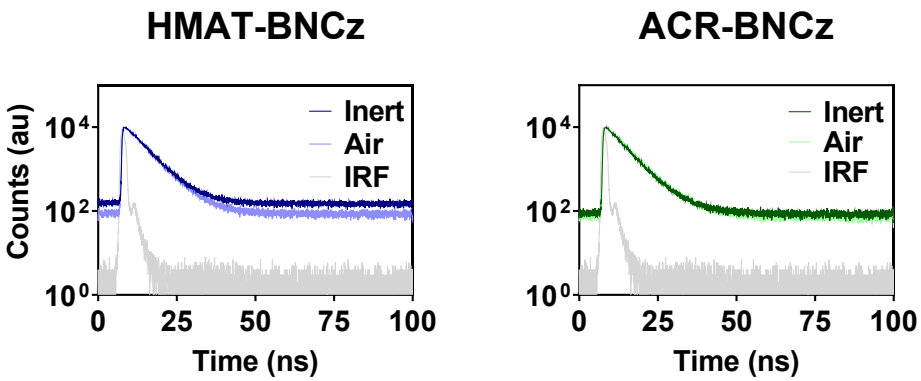

Figure S26. PL decays for 1 wt.% doped mCP films under air or Ar. All measurements were performed using a TCSPC EPLED source with 375 nm excitation.

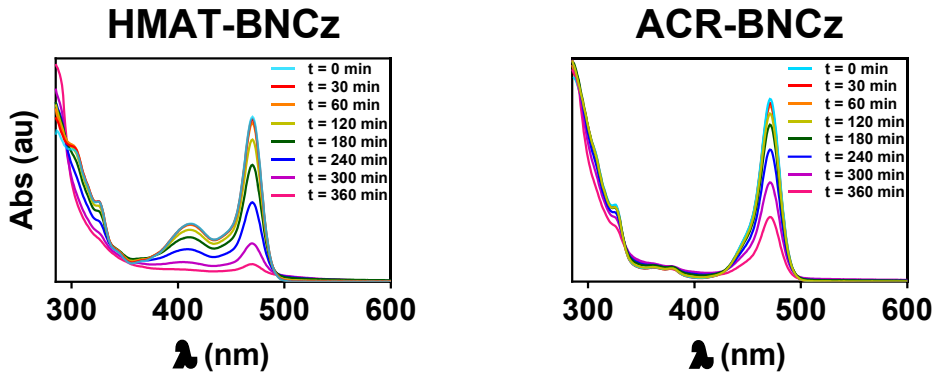

Figure S27. UV-Vis absorption photostability studies for ~10 μM toluene solutions (matched absorbance values at 365 nm) of **HMAT-BNCz** and **ACR-BNCz** using a 365 nm LED. Solutions were irradiated for 30 or 60-minute intervals in cuvettes with stirring, followed by measurement.

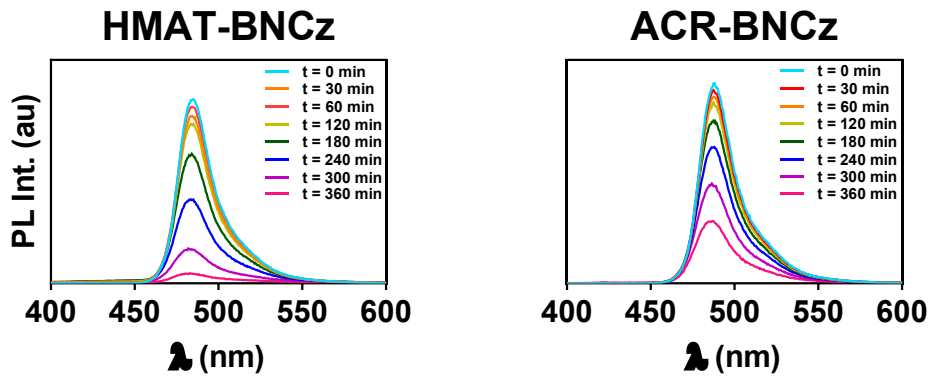

Figure S28. Photoluminescent photostability studies for ~10 μM toluene solutions of **HMAT-BNCz** and **ACR-BNCz** using a 365 nm LED. Solutions were irradiated for 30 or 60-minute intervals in cuvettes with stirring, followed by measurement.

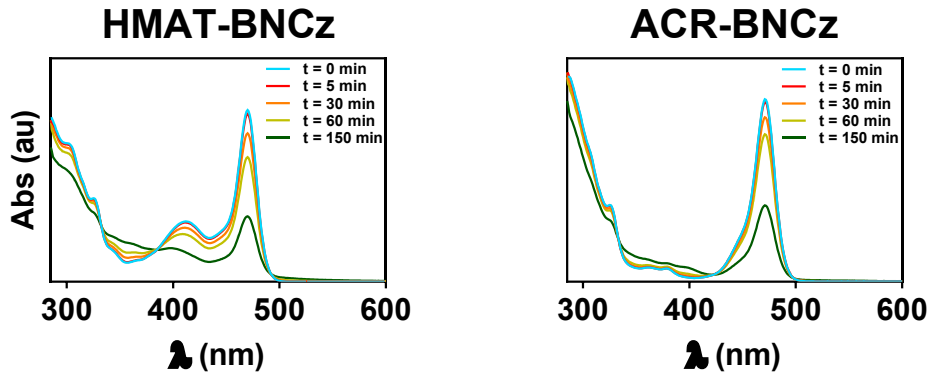

Figure S29. UV-Vis absorption photostability studies for ~10 μM toluene solutions (matched absorbance values at 495 nm) of **HMAT-BNCz** and **ACR-BNCz** using a 450 nm LED. Solutions were irradiated for various time intervals in cuvettes with stirring, followed by measurement.

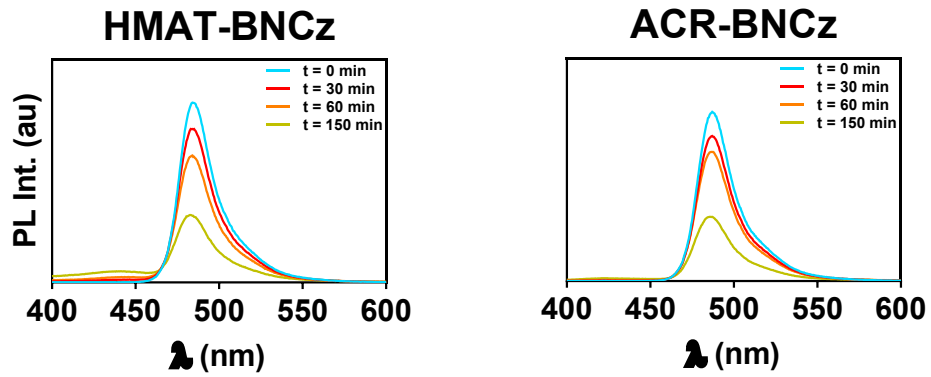

Figure S30. Photoluminescent photostability studies for ~10 μM toluene solutions of **HMAT-BNCz** and **ACR-BNCz** using a 450 nm LED. Solutions were irradiated for various time intervals in cuvettes with stirring, followed by measurement.

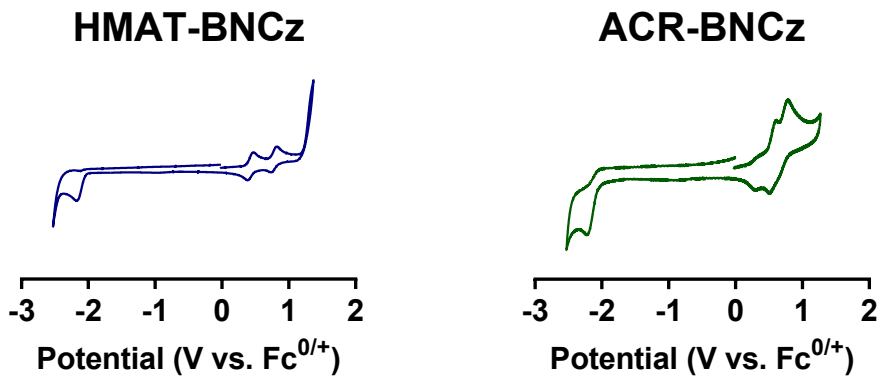

Figure S31. Cyclic voltammograms measured at 2 mM in dry, degassed dichloromethane relative to ferrocene/ferrocenium ($Fc^{0/+}$), with 0.2 M tetrabutylammonium hexafluorophosphate as the electrolyte at a 200 mV/s scan rate. The first anodic and first cathodic peaks were used to calculate experimental HOMO/LUMO values.

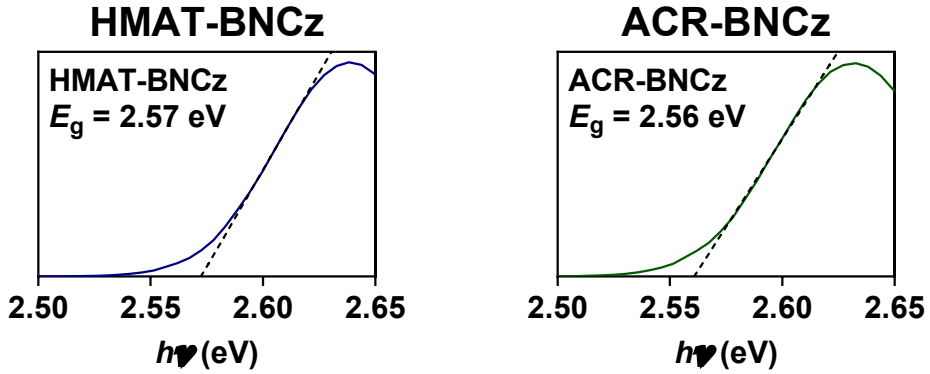

Figure S32. Tauc plots generated from UV-Vis spectra taken in 10 μM toluene solutions.

Table S2. Summarized solid-state emission and lifetime data. Measurements taken as 1 wt.% emitter PMMA films at 298 K. Absolute photoluminescence quantum yields determined using an integrating sphere.

1 wt% PMMA							
Entry	$\lambda_{max,em}$ (nm)	Φ_{air}	CIE (x,y)	τ_p^{air} (ns)	τ_p^{Ar} (ns)	τ_d^{air} (μs)	τ_d^{Ar} (μs)
HMAT-BNCz	486	21.6	(0.112, 0.377)	5.5	5.1	48.2	96.8
ACR-BNCz	485	20.2	(0.102, 0.303)	6.2	6.1	46.9	101.9

Table S3. Summarized solid-state emission and lifetime data. Measurements taken as 1 wt.% emitter Zeonex films at 298 K.

1 wt% Zeonex					
Entry	$\lambda_{max,em}$ (nm)	τ_p^{air} (ns)	τ_p^{Ar} (ns)	τ_d^{air} (μs)	τ_d^{Ar} (μs)
HMAT-BNCz	481	5.0	5.0	12.4	111.1
ACR-BNCz	486	7.6	7.3	20.2	91.9

Table S4. Summarized solid-state emission and lifetime data. Measurements taken as 1 wt.% emitter mCP host films at 298 K.

1 wt% mCP					
Entry	$\lambda_{max,em}$ (nm)	τ_p^{air} (ns)	τ_p^{Ar} (ns)	τ_d^{air} (μs)	τ_d^{Ar} (μs)
HMAT-BNCz	496	5.4	5.5	36.6	71.4
ACR-BNCz	497	5.4	5.4	66.3	80.9

Table S5. Theoretical and experimental electronic properties. [a] HOMO = $-(E_{1/2}^{ox} + 4.8\ eV)$. [b] LUMO = $-(E_{1/2}^{red} + 4.8\ eV)$. [c] Calculated using a Tauc plot of the UV-Vis spectrum in toluene. [d] Determined from onsets of time-gated phosphorescence and fluorescence spectra measured in 2-MeTHF at 77K. [e] Theoretical calculations at the RI-B2PLYP def2-TZVP/C level of theory in toluene using CPCM.

Entry	**HOMO (eV)** [a]	**LUMO (eV)** [b]	E_{gap}^{opt} **(eV)** [c]	ΔE_{ST} **(eV)**	
				Exp. [d]	**Calc.** [e]
HMAT-BNCz	-5.27	-2.63	2.43	0.17	0.10
ACR-BNCz	-5.41	-2.57	2.46	0.16	0.13

Density Functional Theory

Table S6. Results of DFT calculations**.** [a] Calculated at the TPSSH def2-TZVP level of theory in toluene using CPCM. [b] Calculated at the RI-B2PLYP def2-TZVP/C level of theory in toluene using CPCM.

Entry	**HOMO (eV)** [a]	**LUMO (eV)**[a]	E_{gap}^{DFT} **(eV)** [a]	E_{S1} **(eV)** [b]	f [b]		E_{Total} [a] **(10^3 Hartrees)**
					($S_0 \rightarrow S_1$)	**($S_0 \rightarrow S_2$)**	
HMAT-BNCz	-4.75	-2.32	2.57	2.75	0.688	0.666	-3.01
ACR-BNCz	-4.84	-2.38	2.56	2.74	0.710	0.001	-2.78

Table S7. DFT SOC calculations performed at the TPSSH def2-TZVP level of theory in toluene using CPCM.

Entry	S_0-T_1	S_0-T_2	S_1-T_1	S_1-T_2	S_2-T_1	S_2-T_2
HMAT-BNCz	0.18	0.44	0.17	0.03	0.03	0.15
ACR-BNCz	0.50	0.81	0.03	0.13	0.12	0.00

Table S8. Calculated percentage charge-transfer versus locally excited character using interfragment charge transfer method (donors set as one fragment, BNCz-core set as the other) at the RI-B2PLYP def2-TZVP/C level of theory in toluene using CPCM.

Entry	S_1		S_2		S_3		T_1		T_2		T_3	
	% LE	% CT	% LE	% CT	% LE	% CT	% LE	% CT	% LE	% CT	% LE	% CT
HMAT-BNCz	95.2	4.8	38.1	61.9	97.9	2.1	95.9	4.1	49.3	50.7	87.2	12.8
ACR-BNCz	94.7	5.3	46.9	53.1	97.5	2.5	95.9	4.1	98.7	1.3	98.5	1.5

Table S9. Results of DFT calculations**.** [a] Calculated at the TPSSH def2-TZVP level of theory in acetonitrile using CPCM. [b] Calculated at the RI-B2PLYP def2-TZVP/C level of theory in acetonitrile using CPCM.

Entry	HOMO (eV) [a]	LUMO (eV) [a]	E_{S1} (eV) [b]	E_{S2} (eV) [b]	f [b] (S_0→S_1)	f [b] (S_0→S_2)	E_{Total} [a] (10^3 Hartrees)
HMAT-BNCz	-4.79	-2.42	2.75	2.89	0.653	0.647	-3.01
ACR-BNCz	-4.91	-2.46	2.75	3.10	0.680	0.000	-2.78

Table S10. DFT SOC calculations performed at the TPSSH def2-TZVP level of theory in acetonitrile using CPCM.

Entry	S_0-T_1	S_0-T_2	S_1-T_1	S_1-T_2	S_2-T_1	S_2-T_2
HMAT-BNCz	0.45	0.17	0.03	0.17	0.14	0.03
ACR-BNCz	0.46	0.78	0.03	0.12	0.12	0.00

Table S11. Calculated percentage charge-transfer versus locally excited character using interfragment charge transfer method (donors set as one fragment, BNCz-core set as the other) at the RI-B2PLYP def2-TZVP/C level of theory in acetonitrile using CPCM.

Entry	S_1		S_2		S_3		T_1		T_2		T_3	
	% LE	% CT	% LE	% CT	% LE	% CT	% LE	% CT	% LE	% CT	% LE	% CT
HMAT-BNCz	95.6	4.4	36.9	63.1	97.5	2.5	96.0	4.0	49.6	50.4	95.0	5.0
ACR-BNCz	94.8	5.2	44.3	55.7	97.6	2.4	96.0	4.0	98.4	1.6	98.1	1.9

Table S12. Cartesian coordinates [Å] of the optimized structure for **HMAT-BNCz** in toluene.

	X	Y	Z		X	Y	Z
C	-8.189064	-2.905839	2.0241	**C**	-5.420423	-4.157461	0.035847
C	-7.826127	-3.408818	0.607887	**H**	-9.25458	-3.095069	2.235743
C	-8.157749	-4.909706	0.531373	**H**	-8.012417	-1.824088	2.12913
C	-8.693253	-2.668991	-0.436729	**H**	-7.588905	-3.422549	2.789894
C	-6.335764	-3.128926	0.330808	**H**	-9.228676	-5.062454	0.739315
C	-5.863426	-1.800868	0.361652	**H**	-7.5878	-5.492272	1.272659
C	-4.519647	-1.428314	0.128903	**H**	-7.950221	-5.323721	-0.468234
C	-3.654862	-2.504715	-0.141018	**H**	-9.763095	-2.858839	-0.248798
N	-2.28589	-2.420178	-0.391251	**H**	-8.456788	-3.011646	-1.456658
C	-1.585125	-1.209171	-0.27258	**H**	-8.534039	-1.580057	-0.400222
C	-2.343803	0.002473	-0.159269	**H**	-6.585809	-1.012236	0.573445
B	-3.873013	-0.017016	0.08666	**H**	0.219735	3.684711	-0.968605
C	-4.527985	1.373508	0.296088	**H**	0.467287	6.08371	-1.115569
C	-3.67364	2.47768	0.144474	**H**	-3.433626	8.43861	-1.400331
C	-4.108695	3.820334	0.231669	**H**	-2.190803	8.232573	-2.659269
C	-2.949916	4.648604	-0.046211	**H**	-2.295116	9.762949	-1.745158
C	-1.857269	3.769092	-0.287667	**H**	-2.72911	8.523009	1.093988
C	-0.630444	4.304421	-0.695983	**H**	-1.606958	9.849629	0.704881
C	-0.500669	5.695834	-0.796511	**H**	-1.007531	8.382589	1.527664
C	-1.553781	6.588862	-0.515584	**H**	0.29147	8.135036	-2.024283
C	-1.398371	8.117351	-0.615751	**H**	0.778256	8.186193	-0.30646
C	-2.390005	8.66719	-1.666798	**H**	0.088482	9.629814	-1.083195
C	-1.705387	8.752748	0.759845	**H**	-3.650413	6.678798	0.047478
C	0.024253	8.531321	-1.03171	**H**	-5.787529	5.119332	0.594864
C	-2.790852	6.033195	-0.149027	**H**	-7.343958	5.100754	2.261787
C	-5.446505	4.083743	0.518993	**H**	-7.480519	3.581704	3.181295
C	-6.355608	3.018905	0.707448	**H**	-8.949077	4.400103	2.579532
C	-7.828684	3.338015	1.028215	**H**	-7.899119	5.115156	-0.276037

C	-7.901337	4.154202	2.339442	**H**	-9.49124	4.410179	0.092464
C	-8.438211	4.166749	-0.126038	**H**	-8.404151	3.604508	-1.072764
C	-8.677382	2.066661	1.206867	**H**	-8.307814	1.441986	2.035679
C	-5.876773	1.703451	0.584835	**H**	-8.694211	1.453856	0.291439
N	-2.305885	2.434191	-0.122019	**H**	-9.716915	2.34749	1.438631
C	-1.59402	1.224436	-0.148613	**H**	-6.584383	0.887484	0.714849
C	-0.192351	1.220373	-0.105938	**H**	0.354359	2.146591	0.037324
C	0.518827	0.010995	-0.119284	**H**	2.11473	-1.819561	1.114657
C	1.997354	0.005878	-0.010952	**H**	3.161915	-3.650893	0.810811
C	2.688122	-1.018285	0.645572	**H**	4.661017	-4.416941	1.374478
C	4.080281	-1.047773	0.766263	**H**	4.633146	-3.572567	-0.196127
C	4.672791	-2.221053	1.534013	**H**	3.029928	-2.279596	2.999218
C	4.257053	-3.545436	0.837931	**H**	4.412989	-1.26872	3.495534
C	4.127727	-2.202721	2.988111	**H**	4.528777	-3.047007	3.568916
C	4.862477	-0.008636	0.198703	**H**	6.275311	-3.970901	2.687592
N	6.275826	-0.016038	0.302051	**H**	8.752971	-4.015007	2.873917
C	6.933786	-1.077565	0.985928	**H**	10.0593	-2.165482	1.849729
C	6.191903	-2.134284	1.573321	**H**	10.842988	-1.462133	-0.015697
C	6.863773	-3.167617	2.240343	**H**	10.916081	0.063072	-0.924517
C	8.248533	-3.200411	2.350437	**H**	9.670105	-1.149456	-1.322546
C	8.970319	-2.162309	1.774506	**H**	10.679038	-0.136305	2.200373
C	8.347237	-1.104501	1.098208	**H**	9.395859	1.084877	2.407928
C	9.2585	-0.030914	0.521608	**H**	10.753711	1.389671	1.292355
C	10.230972	-0.684726	-0.497455	**H**	6.663783	3.934713	-2.058408
C	10.07114	0.616354	1.675972	**H**	9.142552	3.952198	-1.883435
C	8.452311	1.049434	-0.184476	**H**	10.266544	2.091201	-0.679726
C	7.03728	1.037399	-0.278742	**H**	4.910076	1.252174	-3.128015
C	6.399906	2.10091	-0.967829	**H**	5.054526	3.028869	-3.183146
C	7.172445	3.125941	-1.530461	**H**	3.480425	2.278051	-2.838173
C	8.558811	3.143831	-1.438645	**H**	4.617721	3.558813	0.557166
C	9.178219	2.099224	-0.763739	**H**	3.3076	3.648781	-0.649221
C	4.181885	1.037792	-0.475977	**H**	4.879699	4.400077	-0.993632
C	4.892085	2.203864	-1.149185	**H**	2.295617	1.82768	-1.107343
C	4.564088	2.189723	-2.667056	**H**	0.37246	-2.127516	-0.239216
C	4.394487	3.533429	-0.520161	**H**	0.254394	-3.55079	-1.366521
C	2.78653	1.022193	-0.559012	**H**	0.520769	-5.91582	-1.771036
C	-0.185408	-1.197958	-0.226157	**H**	-2.661132	-8.60618	0.147326
C	-4.079187	-3.848947	-0.20798	**H**	-0.941403	-8.501268	0.598354
C	-2.912528	-4.63273	-0.566459	**H**	-1.52809	-9.874292	-0.380948
C	-1.824584	-3.724278	-0.701757	**H**	-3.361323	-8.258066	-2.325292
C	-0.591659	-4.202155	-1.161782	**H**	-2.210257	-9.526927	-2.808823

C	-0.450929	-5.573082	-1.41393	**H**	-2.117705	-7.905282	-3.550493
C	-1.498571	-6.49942	-1.238229	**H**	0.846093	-8.091949	-1.197892
C	-1.330428	-8.006643	-1.504308	**H**	0.362767	-7.856773	-2.901012
C	-1.635047	-8.790662	-0.207108	**H**	0.169664	-9.447264	-2.129975
C	-2.315111	-8.447084	-2.611864	**H**	-3.59734	-6.666103	-0.701854
C	0.096392	-8.361519	-1.958771	**H**	-5.746564	-5.197258	-0.009197
C	-2.741707	-5.996712	-0.820511				

Table S13. Cartesian coordinates [Å] of the optimized structure for **ACR-BNCz** in toluene.

	X	**Y**	**Z**		**X**	**Y**	**Z**
C	7.519333	-4.331248	1.925533	**C**	2.388944	-5.995412	-0.672067
C	7.43271	-3.407932	0.688307	**C**	5.045862	-4.107164	0.141872
C	8.285951	-2.157027	0.962032	**H**	8.569563	-4.596312	2.131857
C	8.026772	-4.137776	-0.538509	**H**	6.960359	-5.268047	1.775158
C	5.956482	-3.061762	0.413456	**H**	7.108957	-3.831382	2.817324
C	5.475522	-1.741325	0.413089	**H**	9.327737	-2.457413	1.15624
C	4.122857	-1.389376	0.169818	**H**	7.928434	-1.603064	1.844471
C	3.268726	-2.477267	-0.073892	**H**	8.292334	-1.469827	0.101179
N	1.898772	-2.413635	-0.326788	**H**	9.081959	-4.398969	-0.353661
C	1.186749	-1.207785	-0.249374	**H**	7.982411	-3.49837	-1.434463
C	1.933385	0.012106	-0.155247	**H**	7.484848	-5.070264	-0.760737
B	3.464607	0.013481	0.094837	**H**	6.184209	-0.938456	0.604681
C	4.104008	1.41605	0.274559	**H**	-0.655366	3.642173	-1.095617
C	3.240042	2.507548	0.088534	**H**	-0.927328	6.033524	-1.304806
C	3.65953	3.856745	0.144386	**H**	2.205358	8.560946	0.886438
C	2.493929	4.665365	-0.162664	**H**	0.477873	8.411716	1.293191
C	1.412446	3.768791	-0.389374	**H**	1.075878	9.865493	0.446428
C	0.184178	4.27816	-0.825718	**H**	2.954393	8.429617	-1.593144
C	0.040783	5.665	-0.964215	**H**	1.805014	9.729665	-1.989275
C	1.081323	6.576669	-0.696104	**H**	1.736403	8.176754	-2.867868
C	0.909667	8.100281	-0.836154	**H**	-1.272705	8.151272	-0.565248
C	1.18528	8.77141	0.529121	**H**	-0.756155	8.062028	-2.272656
C	1.912653	8.637498	-1.882886	**H**	-0.586246	9.582585	-1.366905
C	-0.510322	8.486609	-1.286297	**H**	3.171773	6.705036	-0.117567
C	2.321059	6.044911	-0.303886	**H**	5.321258	5.182163	0.488308
C	4.991785	4.141471	0.435687	**H**	7.437219	5.182345	-0.362286
C	5.91045	3.091522	0.658944	**H**	7.968046	3.658825	-1.116705
C	7.376453	3.436927	0.985005	**H**	9.034141	4.50637	0.038056

C	7.986272	4.244621	-0.183926	**H**	6.859971	5.22421	2.170064
C	7.426834	4.286083	2.276212	**H**	8.469418	4.549602	2.519908
C	8.23897	2.181374	1.202548	**H**	7.00445	3.729734	3.128058
C	5.447237	1.767948	0.565585	**H**	8.272326	1.546898	0.302766
N	1.874406	2.443403	-0.184101	**H**	7.86923	1.571858	2.042316
C	1.174622	1.228127	-0.169388	**H**	9.272593	2.480985	1.437299
C	-0.226565	1.213022	-0.124111	**H**	6.162435	0.963311	0.722692
C	-0.924807	-0.002249	-0.118765	**H**	-0.785996	2.13974	-0.055419
C	-2.407308	-0.011189	-0.005141	**H**	-2.500347	1.66351	1.369584
C	-3.077221	0.930524	0.801286	**H**	-4.975938	1.649292	1.551756
C	-4.468407	0.921988	0.915005	**H**	-5.693882	1.459673	-1.633465
C	-5.226278	-0.030874	0.221139	**H**	-6.991262	2.808501	-3.238292
N	-6.656092	-0.04284	0.338771	**H**	-9.502458	2.85059	-3.09886
C	-7.423786	0.715446	-0.560107	**H**	-10.635338	1.529199	-1.343273
C	-6.781729	1.472578	-1.565875	**H**	-11.154724	1.484924	0.818015
C	-7.517119	2.234016	-2.471637	**H**	-9.792305	1.642048	1.959095
C	-8.912398	2.258651	-2.395969	**H**	-11.029588	0.380934	2.206988
C	-9.544129	1.509292	-1.401294	**H**	-11.267582	-0.53325	-0.778241
C	-8.835509	0.730837	-0.472111	**H**	-11.144562	-1.637018	0.611465
C	-9.608795	-0.062718	0.587481	**H**	-9.985023	-1.772741	-0.737588
C	-10.44659	0.921467	1.445242	**H**	-5.357558	-1.528069	2.123127
C	-10.55867	-1.062584	-0.122782	**H**	-6.350011	-2.888542	3.923004
C	-8.658546	-0.841597	1.504412	**H**	-8.848294	-2.962206	4.207121
C	-7.252455	-0.808295	1.354494	**H**	-10.276514	-1.659939	2.665751
C	-6.441096	-1.554574	2.238594	**H**	-5.168573	-1.708469	-1.134452
C	-7.004417	-2.322733	3.255268	**H**	-2.695552	-1.687122	-1.350893
C	-8.39218	-2.364868	3.414801	**H**	-0.763349	-2.142854	-0.144345
C	-9.191376	-1.626214	2.539855	**H**	-0.631558	-3.592074	-1.263836
C	-4.575916	-0.972962	-0.586946	**H**	-0.875637	-5.968945	-1.617389
C	-3.184237	-0.96171	-0.696584	**H**	3.031393	-8.285832	-2.120348
C	-0.215812	-1.208241	-0.207346	**H**	1.786433	-7.973789	-3.355313
C	3.705629	-3.821541	-0.108963	**H**	1.892934	-9.576296	-2.575133
C	2.546071	-4.624803	-0.449795	**H**	2.330326	-8.582022	0.359045
C	1.450493	-3.73037	-0.606104	**H**	1.209762	-9.872545	-0.140638
C	0.221797	-4.23059	-1.051318	**H**	0.608929	-8.482242	0.80506
C	0.093768	-5.608242	-1.272132	**H**	-0.695579	-7.932141	-2.71028
C	1.150388	-6.519838	-1.077512	**H**	-1.179384	-8.133494	-1.002753
C	0.996725	-8.034267	-1.308296	**H**	-0.488671	-9.502754	-1.903109
C	1.987401	-8.491205	-2.403759	**H**	3.250852	-6.65364	-0.538027
C	1.3065	-8.784226	0.007716	**H**	5.388099	-5.144882	0.122763
C	-0.425994	-8.412814	-1.756395				

Table S14. Cartesian coordinates [Å] of the optimized structure for **HMAT-BNCz** in acetonitrile.

	X	Y	Z		X	Y	Z
C	-8.19784	-2.899581	2.013055	**C**	-5.424633	-4.156193	0.035216
C	-7.831814	-3.404338	0.598119	**H**	-9.264043	-3.088334	2.220568
C	-8.163913	-4.905051	0.520907	**H**	-8.021355	-1.817663	2.117489
C	-8.69487	-2.662995	-0.448971	**H**	-7.601518	-3.417916	2.781022
C	-6.34037	-3.125829	0.325364	**H**	-9.235665	-5.055713	0.725355
C	-5.866699	-1.797847	0.355903	**H**	-7.596969	-5.487914	1.264192
C	-4.520798	-1.427252	0.127326	**H**	-7.953108	-5.319682	-0.477706
C	-3.655552	-2.504847	-0.139147	**H**	-9.764838	-2.853244	-0.26344
N	-2.285534	-2.42241	-0.385982	**H**	-8.456684	-3.006917	-1.468282
C	-1.584549	-1.210621	-0.272566	**H**	-8.536071	-1.573978	-0.410809
C	-2.344268	0.001564	-0.161897	**H**	-6.589522	-1.008619	0.563626
B	-3.8728	-0.016643	0.086596	**H**	0.213673	3.682898	-1.008401
C	-4.526649	1.373999	0.299074	**H**	0.459333	6.079315	-1.162504
C	-3.67239	2.477853	0.140142	**H**	-3.445015	8.438233	-1.412654
C	-4.106836	3.821052	0.227677	**H**	-2.214745	8.229153	-2.685586
C	-2.949402	4.64892	-0.059854	**H**	-2.307734	9.759812	-1.771712
C	-1.858493	3.768877	-0.30754	**H**	-2.714886	8.525003	1.071948
C	-0.634717	4.301764	-0.728565	**H**	-1.595648	9.849912	0.668478
C	-0.506008	5.693431	-0.833548	**H**	-0.987344	8.385608	1.48856
C	-1.556933	6.587747	-0.545401	**H**	0.274158	8.128794	-2.076215
C	-1.401141	8.11593	-0.650187	**H**	0.778875	8.183096	-0.36398
C	-2.404057	8.664514	-1.691299	**H**	0.08099	9.625749	-1.135881
C	-1.694224	8.75344	0.727613	**H**	-3.65003	6.679673	0.034791
C	0.017491	8.527448	-1.081838	**H**	-5.782263	5.122107	0.599018
C	-2.791969	6.033954	-0.167214	**H**	-7.330628	5.111265	2.270896
C	-5.442965	4.086154	0.523212	**H**	-7.460682	3.595219	3.199336
C	-6.351547	3.021313	0.720049	**H**	-8.93253	4.409745	2.602007
C	-7.822504	3.341568	1.049406	**H**	-7.900036	5.113797	-0.261558
C	-7.886008	4.164298	2.357156	**H**	-9.489613	4.410409	0.12091
C	-8.438474	4.166154	-0.104594	**H**	-8.412607	3.598949	-1.048848
C	-8.669668	2.070803	1.238957	**H**	-8.294337	1.448618	2.067054
C	-5.874229	1.704956	0.596877	**H**	-8.693697	1.454211	0.326279
N	-2.306366	2.43347	-0.134884	**H**	-9.706953	2.353857	1.477339
C	-1.593852	1.224022	-0.157243	**H**	-6.581951	0.890218	0.73447
C	-0.192178	1.220965	-0.1161	**H**	0.352874	2.149498	0.018256
C	0.520466	0.011455	-0.125822	**H**	2.123899	-1.865411	1.033404
C	1.999238	0.006617	-0.016175	**H**	3.181615	-3.678399	0.637981
C	2.69283	-1.04179	0.599493	**H**	4.680432	-4.461834	1.178576

C	4.085011	-1.071834	0.72084	**H**	4.659545	-3.547598	-0.353344
C	4.68	-2.276104	1.437163	**H**	3.029788	-2.413651	2.888044
C	4.275917	-3.569404	0.678256	**H**	4.403277	-1.417034	3.43937
C	4.126938	-2.328499	2.887388	**H**	4.529312	-3.19683	3.430261
C	4.86492	-0.006762	0.198838	**H**	6.28657	-4.062071	2.530513
N	6.277584	-0.01464	0.302651	**H**	8.763911	-4.104279	2.719916
C	6.938438	-1.101821	0.943452	**H**	10.066913	-2.215523	1.766394
C	6.198485	-2.183005	1.487934	**H**	10.838837	-1.448041	-0.089332
C	6.872488	-3.239601	2.116233	**H**	10.90982	0.110837	-0.938445
C	8.257755	-3.271812	2.227168	**H**	9.657939	-1.082839	-1.376095
C	8.978023	-2.210884	1.691033	**H**	10.696942	-0.208906	2.17352
C	8.352299	-1.129597	1.054236	**H**	9.417266	1.005308	2.441131
C	9.261698	-0.035846	0.513487	**H**	10.766507	1.350352	1.325799
C	10.225559	-0.651725	-0.53713	**H**	6.65623	4.037008	-1.885187
C	10.085357	0.564552	1.685301	**H**	9.135686	4.045497	-1.721296
C	8.452603	1.072436	-0.14437	**H**	10.265219	2.135364	-0.603159
C	7.037064	1.063938	-0.234983	**H**	4.889519	1.434261	-3.072965
C	6.396288	2.155828	-0.875394	**H**	5.035866	3.211731	-3.02405
C	7.166458	3.205219	-1.39608	**H**	3.464326	2.445431	-2.71258
C	8.553766	3.218664	-1.309338	**H**	4.629396	3.523404	0.742627
C	9.176628	2.146164	-0.681962	**H**	3.306384	3.680508	-0.443715
C	4.181499	1.066144	-0.430882	**H**	4.874635	4.451813	-0.761161
C	4.887388	2.268786	-1.041448	**H**	2.296596	1.87664	-1.032808
C	4.548671	2.343885	-2.555091	**H**	0.372706	-2.127897	-0.240444
C	4.394549	3.559569	-0.332232	**H**	0.261945	-3.566176	-1.340153
C	2.786403	1.048462	-0.519235	**H**	0.522224	-5.930173	-1.736884
C	-0.184731	-1.198316	-0.229133	**H**	-2.669077	-8.605188	0.178986
C	-4.081928	-3.848776	-0.20475	**H**	-0.947831	-8.501551	0.630634
C	-2.914961	-4.635452	-0.557277	**H**	-1.537178	-9.877302	-0.342429
C	-1.824559	-3.729348	-0.690571	**H**	-3.367213	-8.270829	-2.294116
C	-0.589653	-4.211786	-1.141351	**H**	-2.216009	-9.54217	-2.770525
C	-0.451369	-5.584356	-1.388201	**H**	-2.121796	-7.92569	-3.521946
C	-1.502596	-6.508017	-1.215785	**H**	0.840575	-8.103529	-1.165912
C	-1.335709	-8.01663	-1.474608	**H**	0.359058	-7.873537	-2.870166
C	-1.642781	-8.792995	-0.1732	**H**	0.161973	-9.461153	-2.093401
C	-2.321059	-8.461399	-2.579969	**H**	-3.605222	-6.667838	-0.688717
C	0.091125	-8.37471	-1.926436	**H**	-5.751004	-5.195851	-0.009065
C	-2.747257	-6.00138	-0.805944				

Table S15. Cartesian coordinates [Å] of the optimized structure for **ACR-BNCz** in acetonitrile.

	X	Y	Z		X	Y	Z
C	7.512941	-4.330959	1.940769	**C**	2.391212	-5.998026	-0.667738
C	7.430874	-3.408699	0.702291	**C**	5.045009	-4.10876	0.149842
C	8.283693	-2.157588	0.976334	**H**	8.562621	-4.596003	2.1489
C	8.026938	-4.141401	-0.521989	**H**	6.953831	-5.267527	1.789653
C	5.955466	-3.062638	0.422919	**H**	7.102461	-3.828745	2.831444
C	5.474824	-1.741724	0.42004	**H**	9.324347	-2.459377	1.173628
C	4.122078	-1.389605	0.172569	**H**	7.924328	-1.601823	1.856928
C	3.267666	-2.477761	-0.071865	**H**	8.292988	-1.471541	0.11457
N	1.898276	-2.414265	-0.32762	**H**	9.081094	-4.402709	-0.332665
C	1.185496	-1.208404	-0.249315	**H**	7.987259	-3.502449	-1.418734
C	1.932571	0.012006	-0.152967	**H**	7.48488	-5.073909	-0.743663
B	3.463799	0.013169	0.094767	**H**	6.183863	-0.93959	0.613671
C	4.10506	1.415561	0.268476	**H**	-0.668151	3.652834	-1.060994
C	3.239777	2.507519	0.087188	**H**	-0.934511	6.041704	-1.267148
C	3.661469	3.856468	0.140024	**H**	2.227951	8.563923	0.890895
C	2.494413	4.666657	-0.158496	**H**	0.503095	8.419254	1.316843
C	1.409737	3.77165	-0.377444	**H**	1.095967	9.870048	0.462214
C	0.177906	4.283982	-0.801151	**H**	2.94976	8.429952	-1.594358
C	0.03663	5.67174	-0.93708	**H**	1.798512	9.732141	-1.978407
C	1.081839	6.581571	-0.678389	**H**	1.716786	8.180604	-2.857429
C	0.911745	8.105524	-0.81686	**H**	-1.267674	8.160209	-0.523252
C	1.204167	8.776044	0.545337	**H**	-0.769186	8.070411	-2.235823
C	1.905624	8.639899	-1.87388	**H**	-0.585692	9.590525	-1.33133
C	-0.512185	8.494382	-1.252054	**H**	3.178282	6.704846	-0.116552
C	2.32437	6.047387	-0.296917	**H**	5.325744	5.182072	0.470879
C	4.996261	4.141413	0.421352	**H**	7.435704	5.177431	-0.400294
C	5.916427	3.090503	0.638018	**H**	7.961348	3.650548	-1.155106
C	7.385293	3.435173	0.951771	**H**	9.035053	4.500946	-0.010276
C	7.985611	4.239761	-0.224387	**H**	6.879628	5.227337	2.134614
C	7.445952	4.288798	2.239721	**H**	8.490921	4.551417	2.473084
C	8.248091	2.179288	1.166074	**H**	7.031465	3.734739	3.097185
C	5.451535	1.766846	0.549203	**H**	8.274769	1.542471	0.267719
N	1.872372	2.444405	-0.177126	**H**	7.884151	1.571863	2.009921
C	1.172808	1.228436	-0.164555	**H**	9.283143	2.479837	1.392551
C	-0.228339	1.212385	-0.12051	**H**	6.168088	0.962349	0.701065
C	-0.926753	-0.003351	-0.118846	**H**	-0.78886	2.138102	-0.050941
C	-2.409801	-0.012076	-0.006761	**H**	-2.506447	1.682685	1.345604
C	-3.080304	0.939874	0.787481	**H**	-4.978154	1.667764	1.528141
C	-4.471595	0.931605	0.90094	**H**	-5.695622	1.445917	-1.648756

C	-5.227615	-0.030588	0.218007	**H**	-6.992429	2.781909	-3.264353
N	-6.658415	-0.041952	0.335175	**H**	-9.504717	2.824251	-3.126562
C	-7.426032	0.708671	-0.569823	**H**	-10.63843	1.515973	-1.361694
C	-6.783507	1.458433	-1.58149	**H**	-11.155407	1.490758	0.80507
C	-7.518781	2.213046	-2.493879	**H**	-9.790448	1.654633	1.943189
C	-8.914707	2.23777	-2.419033	**H**	-11.029694	0.396517	2.201058
C	-9.547244	1.495471	-1.418686	**H**	-11.274884	-0.535944	-0.775726
C	-8.838353	0.724247	-0.482929	**H**	-11.15255	-1.629357	0.621066
C	-9.612266	-0.060398	0.582964	**H**	-9.995311	-1.779235	-0.729324
C	-10.446889	0.931359	1.4353	**H**	-5.360363	-1.515571	2.130252
C	-10.565965	-1.062807	-0.118535	**H**	-6.353633	-2.866185	3.937185
C	-8.661988	-0.834696	1.503881	**H**	-8.853062	-2.940279	4.219145
C	-7.255247	-0.801244	1.354639	**H**	-10.28091	-1.647666	2.668987
C	-6.444045	-1.541788	2.244578	**H**	-5.166952	-1.725967	-1.117868
C	-7.007914	-2.304781	3.265603	**H**	-2.698178	-1.707054	-1.331617
C	-8.396411	-2.347158	3.423944	**H**	-0.764815	-2.144257	-0.153846
C	-9.195778	-1.613885	2.543584	**H**	-0.632478	-3.597507	-1.268588
C	-4.577033	-0.982359	-0.578496	**H**	-0.873003	-5.972313	-1.619404
C	-3.185119	-0.972144	-0.687188	**H**	3.039542	-8.293192	-2.102029
C	-0.217058	-1.209362	-0.20934	**H**	1.801132	-7.983304	-3.346287
C	3.705131	-3.822311	-0.104418	**H**	1.901717	-9.582937	-2.56047
C	2.546079	-4.626348	-0.446854	**H**	2.324425	-8.580811	0.372405
C	1.450368	-3.732363	-0.606523	**H**	1.206671	-9.872501	-0.131044
C	0.222256	-4.233129	-1.053611	**H**	0.598852	-8.481462	0.808318
C	0.09589	-5.611642	-1.272878	**H**	-0.685053	-7.936731	-2.714851
C	1.152962	-6.52295	-1.075146	**H**	-1.178265	-8.135377	-1.009932
C	0.999667	-8.0378	-1.303603	**H**	-0.481959	-9.506379	-1.903901
C	1.997112	-8.497669	-2.391816	**H**	3.253494	-6.655052	-0.531027
C	1.302458	-8.784112	0.016265	**H**	5.386193	-5.146706	0.132607
C	-0.420787	-8.41622	-1.758889				

Single Crystal X-ray Diffraction

Table S16: X-ray crystallographic data for **HMAT-BNCz** and **ACR-BNCz**.

Compound	**HMAT-BNCz**	**ACR-BNCz**
Formula	$C_{73}H_{74}BN_3$	$C_{67}H_{66}BN_3$
$D_{calc.}$/g/cm^3	1.048	1.178
μ/mm^{-1}	0.451	0.509
Formula weight	1004.16	924.03
Colour	Light yellow	Light Yellow
Shape	Plate	Needle
Size/mm^3	0.31 × 0.21 × 0.05	0.21 × 0.16 × 0.15
Temperature/K	100	100
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	15.0601(3)	5.7620(3)
b/Å	15.8549(3)	17.6427(9)
c/Å	15.9070(3)	26.8801(12)
α/°	64.9470(10)	74.680(4)
β/°	67.9500(10)	85.587(3)
γ/°	84.0660(10)	81.527(4)
Volume/Å^3	3182.19(11)	2604.6(2)
Z	2	2
Z'	1	1
Wavelength/ Å	1.54178	1.54178
Radiation type	Cu K_α	Cu K_α
Θ_{min}/°	3.173	2.620
Θ_{max}/°	77.157	61.150
Measured reflections	78108	43389
Independent reflections	13389	8056
Reflections I≥2 σ(I)	12237	5721
R_{int}	0.0347	0.0885
Parameters	712	703
Restraints	0	720
Largest peak	0.411	0.20
Deepest hole	-0.320	-0.23
GooF	1.033	1.005
wR_2 (all data)	0.1134	0.1406
wR_2	0.1103	0.1235
R_1 (all data)	0.0445	0.0785
R_1	0.0411	0.0505

Crystallographic details: Single crystals of **HMAT-BNCz** and **ACR-BNCz** were recrystallised from a mixture of DCM and *n*-hexanes by slow evaporation. A suitable crystal was selected and mounted onto a mylar loop in oil, then placed on a Bruker D8 Venture Photon III Area Detector. The crystal was kept at a steady T = 100.0 K during data collection. Structural solutions were obtained using ShelXT 2018/2 program using Intrinsic Phasing methods and by using Olex2 1.5 as the graphical interface.[1,2] The model was refined with XL using full matrix least squares minimization on F^2. The structure was solved and the space group P-1 (No. 2) determined by the ShelXT 2018/2 structure solution program using Intrinsic phasing methods and refined by full matrix least squares minimization on F^2 using version 2018/3 of XL.[3] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. The SQUEEZE function in PLATON was used to deal with a co-crystallized *n*-hexane solvent molecule which was disordered and could not be modelled properly.[4]

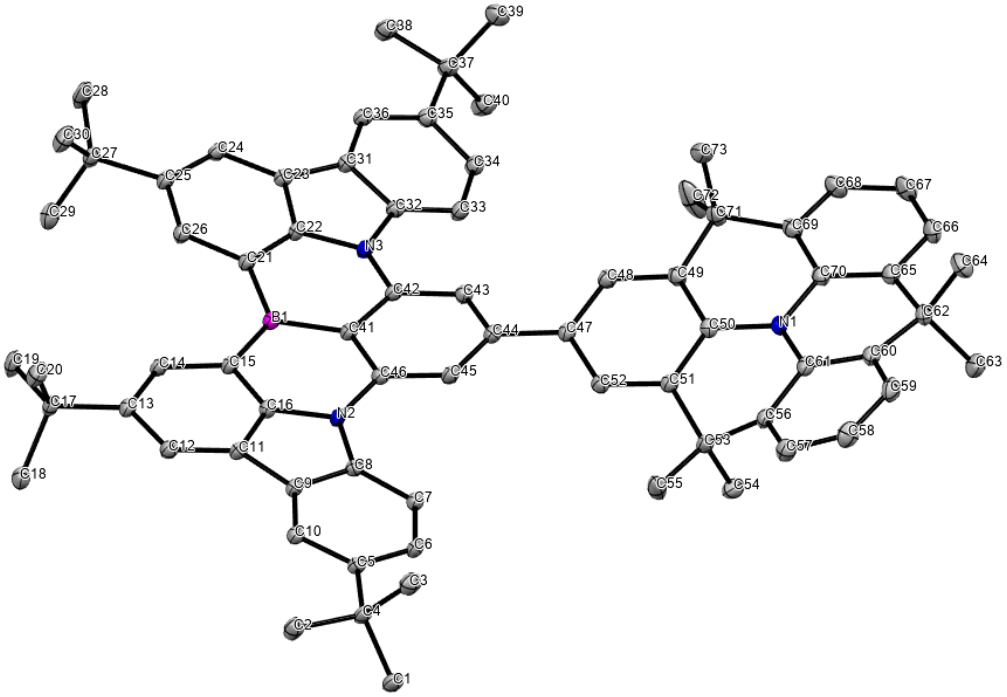

Figure S33: ORTEP-style image of **HMAT-BNCz**. Hydrogen atoms removed for clarity. Grey: carbon, blue: nitrogen, magenta: boron.

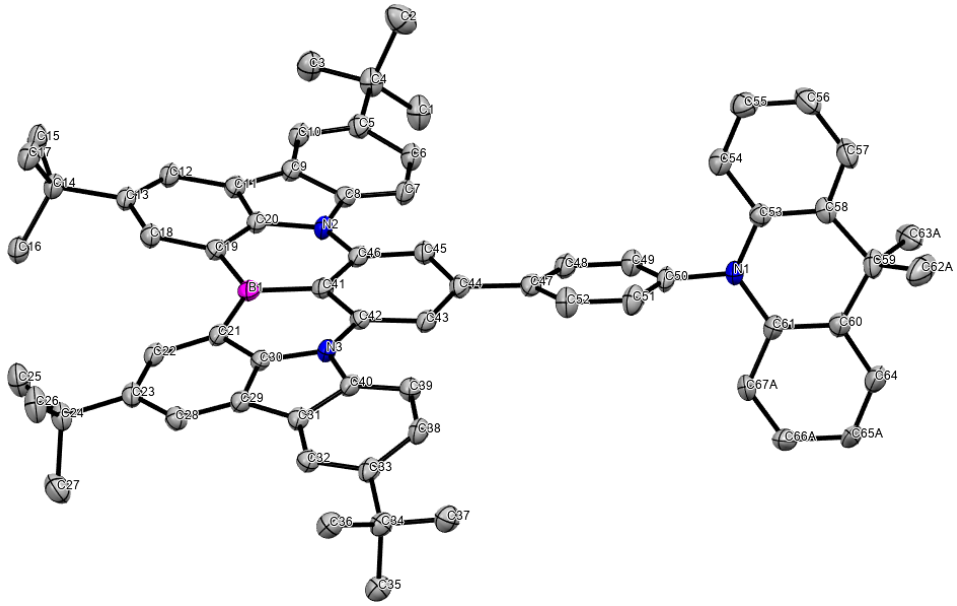

Figure S34: ORTEP-style image of ACR-BNCz. Hydrogen atoms and minor disordered fragments were removed for clarity. Grey: carbon, blue: nitrogen, magenta: boron.

References:

1. G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Adv.,* 2015, **71**, 3.

2. G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.,* 2015, **71**, 3.

3. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.,* 2009, **42**, 339.

4. A. L. Spek, *Acta Crystallogr. Sect. C Struct. Chem.,* 2015, **71**, 9.

5. M. D. Hanwell, D. E. Curtis, D. C. Lonie, T. Vandermeerschd, E. Zurek and G. R. Hutchison, *J. Cheminform.,* 2012, **4**, 1.

6. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K.

Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, *Gaussian 16 Revision B.01.,* Gaussian, Inc: Wallingford CT **2016**.

7. F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.,* 2012, **2**, 73.

8. F. Neese, *Wiley Interdiscip. Rev. Comput. Mol. Sci.,* 2022, **12**, e1606.

9. T. Lu and F. Chen, *J. Comput. Chem.,* 2012, **33**, 580.

10. Z. Liu, T. Lu and Q. Chen, *Carbon,* 2020, *165*, 461.

11. K. Momma and F. Izumi, *J. Appl. Crystallogr.,* 2011, **44**, 1272.

12. S. Grimme and F. Neese, *J. Chem. Phys.,* 2007, **127**, 154116.

13. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.,* 2005, **7**, 3297.

14. M. J. G. Peach, M.J. Williamson and D.J. Tozer *J. Chem. Theory Comput.,* 2011, **7**, 3578−3585.