Supporting Information

Enhancing OLED Emitter Efficiency through Increased Rigidity

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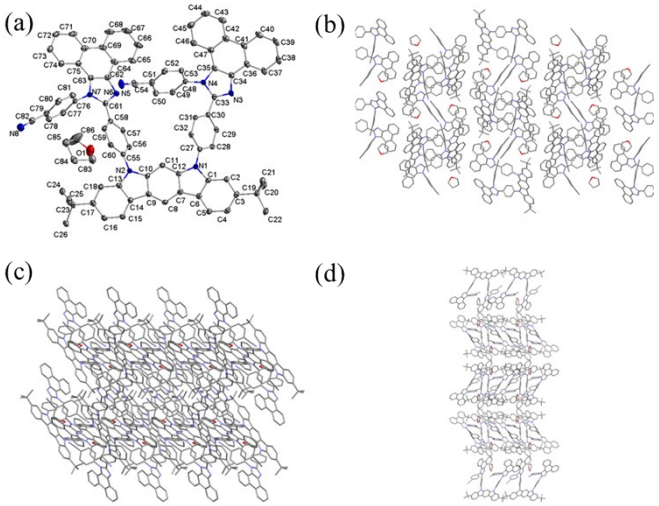

Figure S1. (a) Single crystal structure of CN-PAI-InCz·THF with number of carbon and nitrogen, (b)-(d) intermolecular packing geometries of CN-PAI-InCz·THF in the single crystal determined by XRD analysis: (b) a-axis view, (c) b-axis view, (d) c-axis view.

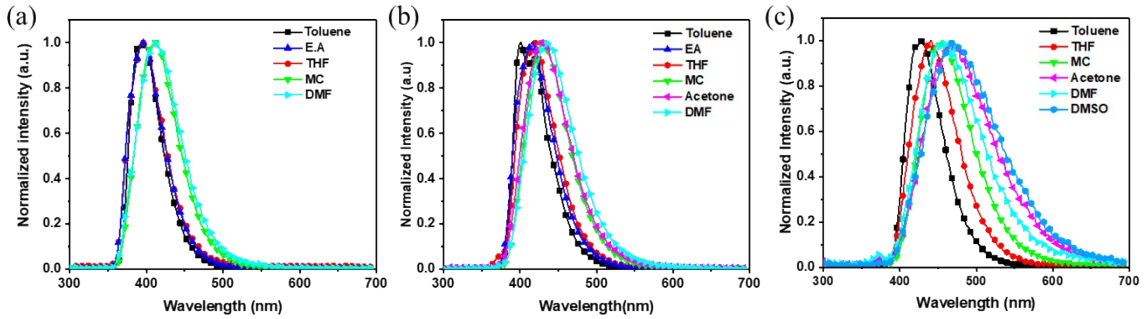

Fig S2. PL spectra depend on the various polarity solvents (a) TPI-InCz, (b) PAI-InCz, (c) CN-PAI-InCz

Table S1. PLmax according to various polarity solvents

	PLmax (nm)						
	Toluene (2.38)[a]	EA (6.02)	THF (7.58)	MC (8.93)	Acetone (20.7)	DMF (36.7)	DMSO (46.7)
TPI-InCz	390	396	394	408	N/A	412	N/A
PAI-InCz	400,417	415	419	427	427	435	N/A
CN-PAI-InCz	430	N/A[b]	441	454	459	465	470

[a]dielectric constant of solvent, [b]N/A: not available due to low solubility.

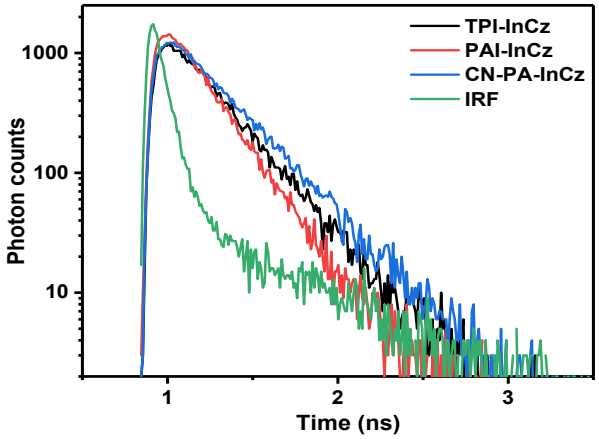

Fig S3. TRPL of synthesized materials in solution state.

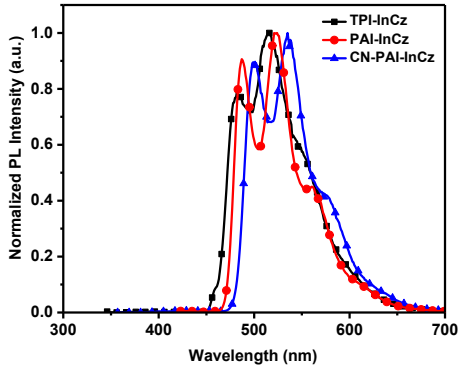

Fig S4. Low temperature PL (LTPL) spectra at 77K in solution state.

Table S2. Energy levels of synthesized materials in solution state.

	S_1 (eV)	T_1 (eV)	ΔE_{ST} (eV)
TPI-InCz	3.17	2.68	0.49
PAI-InCz	3.10	2.62	0.48
CN-PAI-InCz	2.88	2.58	0.30

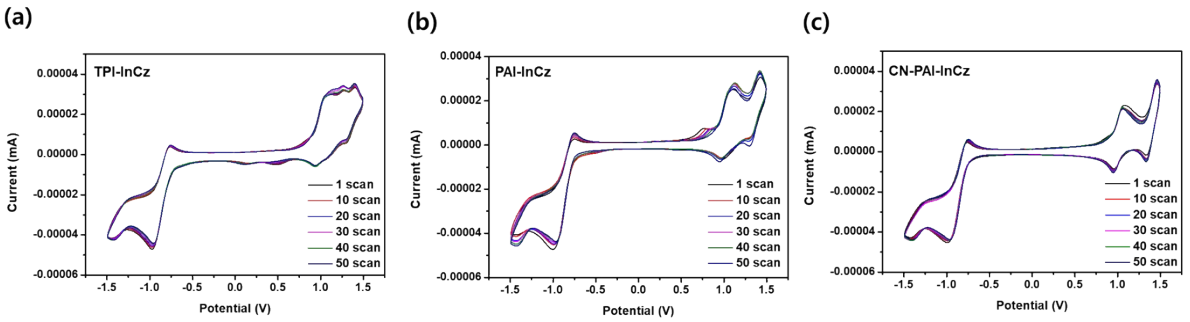

Fig S5. The consecutive CV scans up to 50 cycles of (a) TPI-InCz, (b) PAI-InCz and (c) CN-PAI-InCz (solvent: MC, electrolyte: 0.1M TBAP-F_6, scan rate: 100 mV/s).

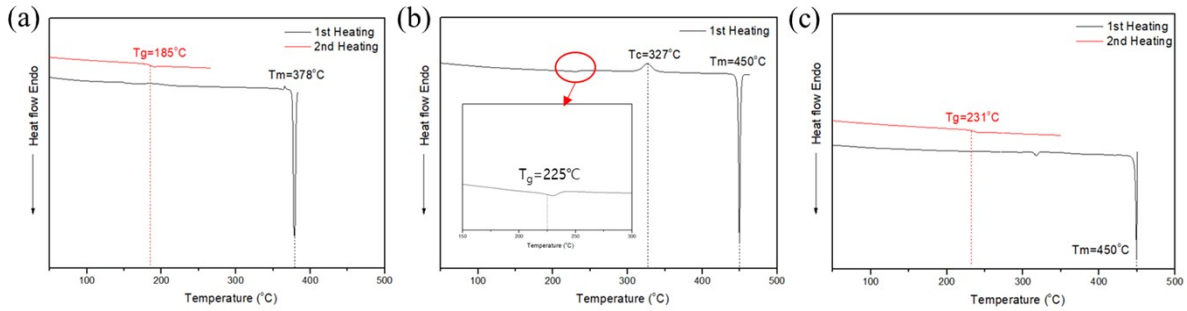

Fig S6. DSC curves (a) TPI-InCz, (b) PAI-InCz and (c) CN-PAI-InCz

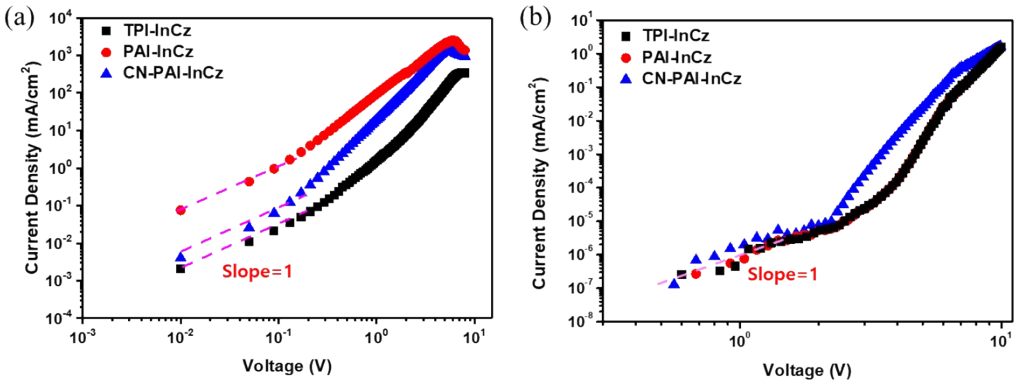

Fig S7. (a) J-V characteristics of HOD, (b) J-V characteristics of EOD

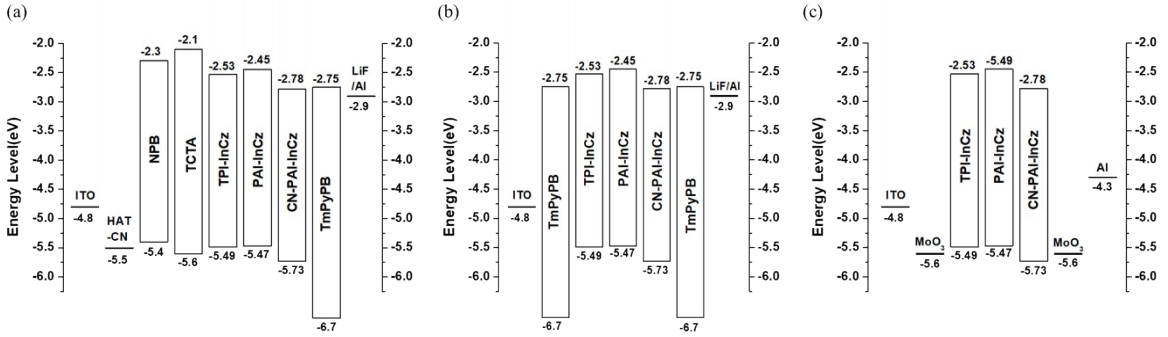

Fig S8. Band diagrams of (a) non-doped OLED device, (b) HOD, (c) EOD.

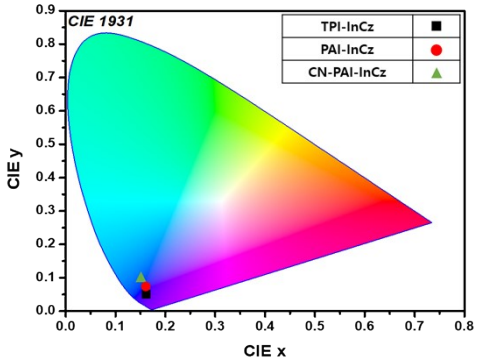

Fig S9. CIE diagram of non-doped OLED devices.

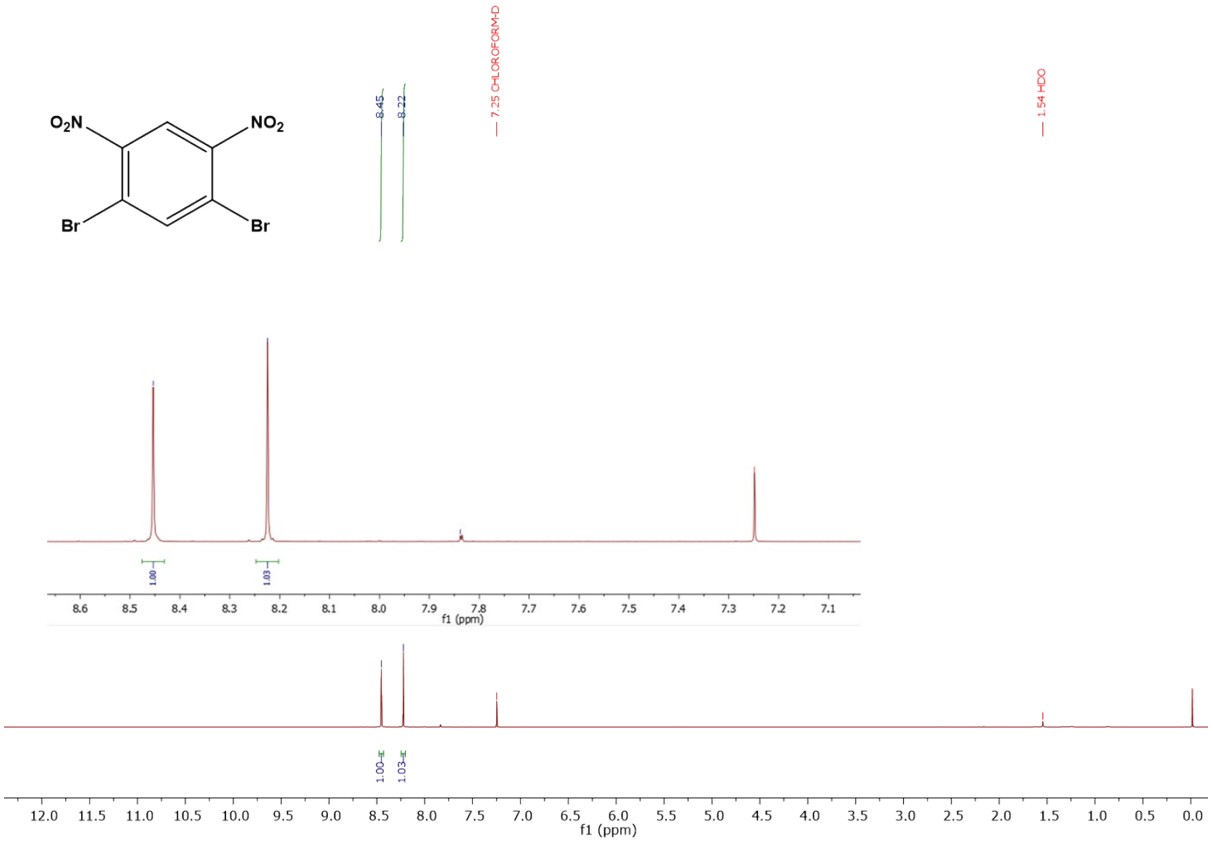

Figure S10. ^{1}H NMR spectra of compound (1) in $CDCl_3$.

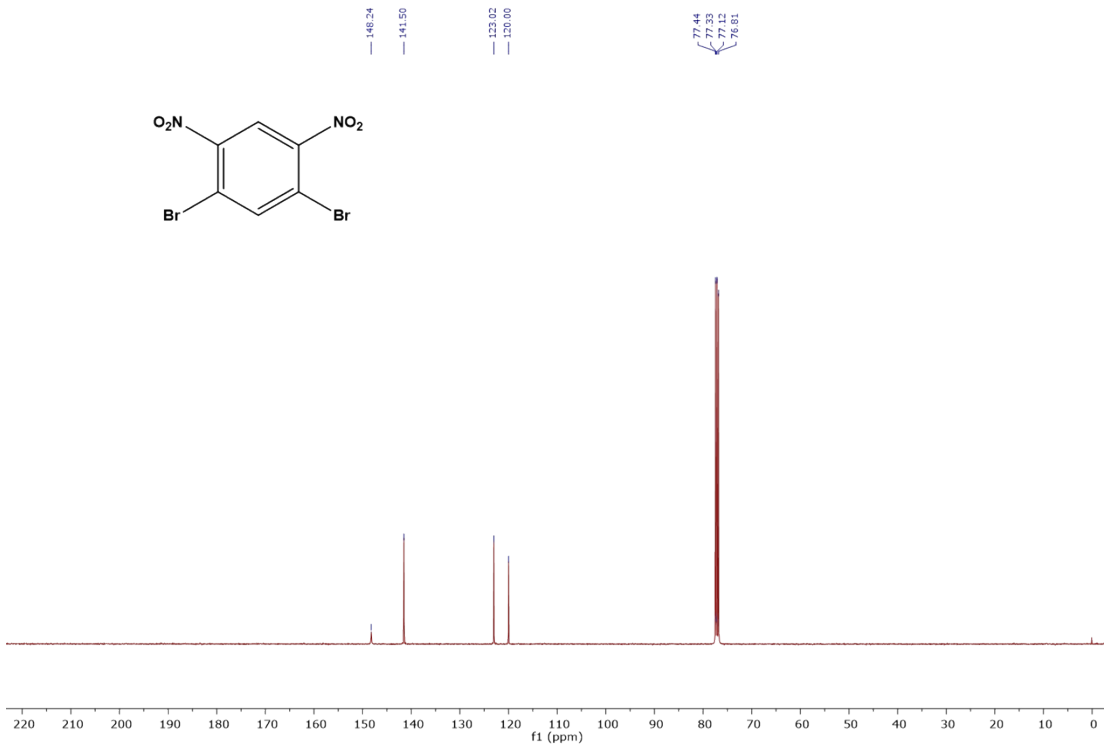

Figure S11. ^{13}C NMR spectra of compound (1) in $CDCl_3$.

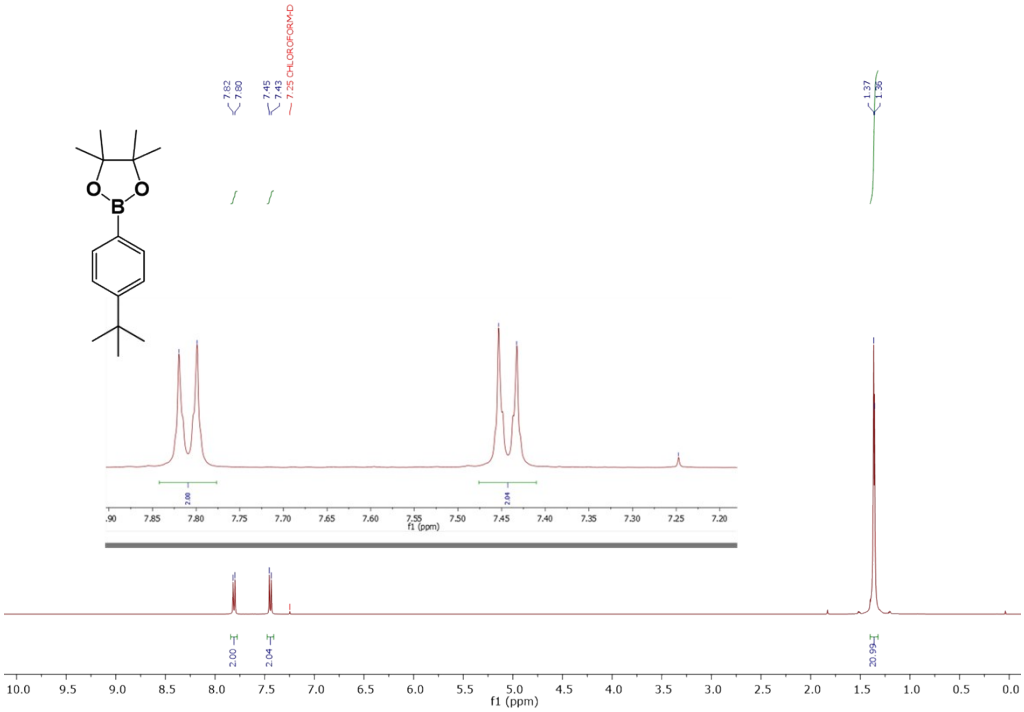

Figure S12. ^{1}H NMR spectra of compound (2) in $CDCl_3$.

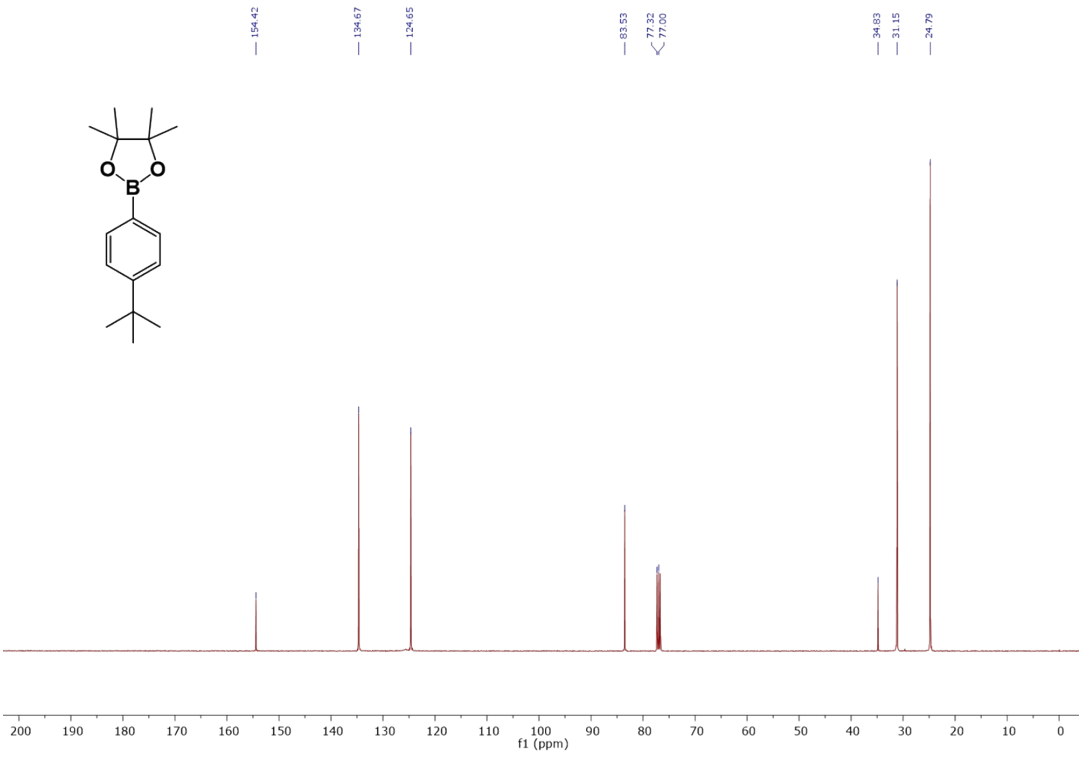

Figure S13. ^{13}C NMR Spectra of compound (2) in $CDCl_3$.

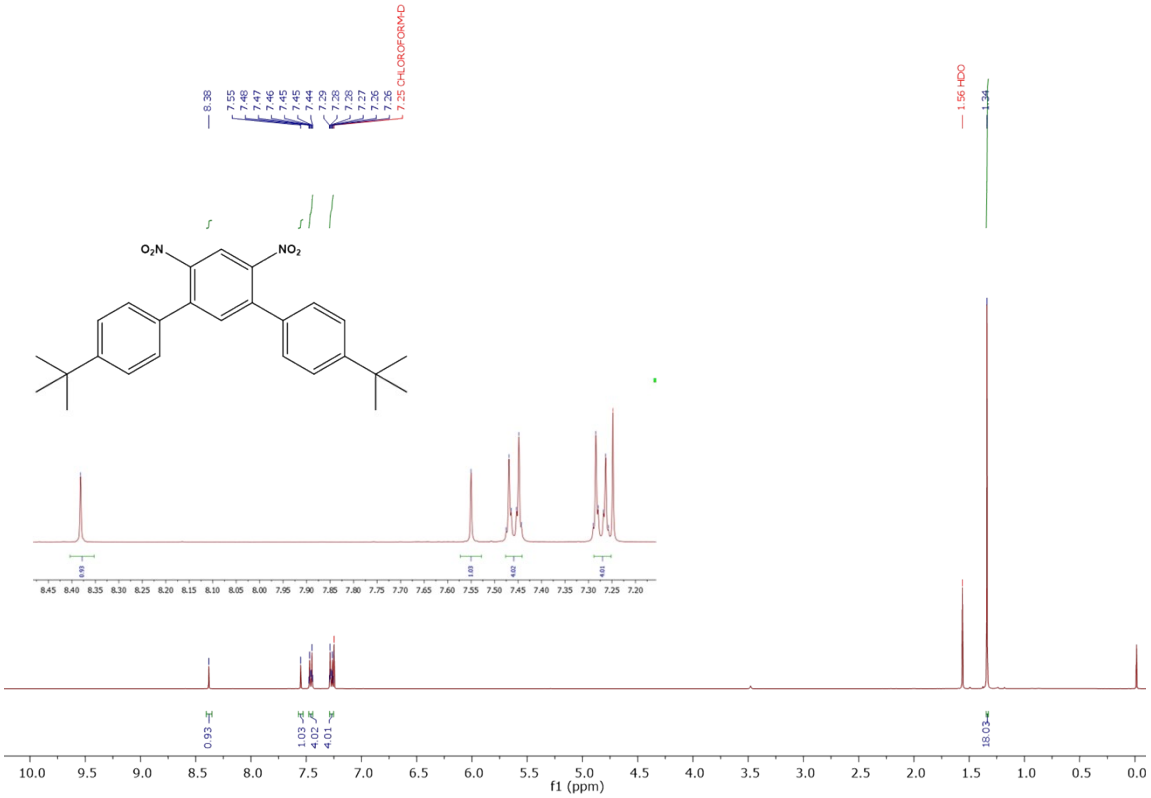

Figure S14. ^{1}H NMR spectra of compound (3) in $CDCl_3$.

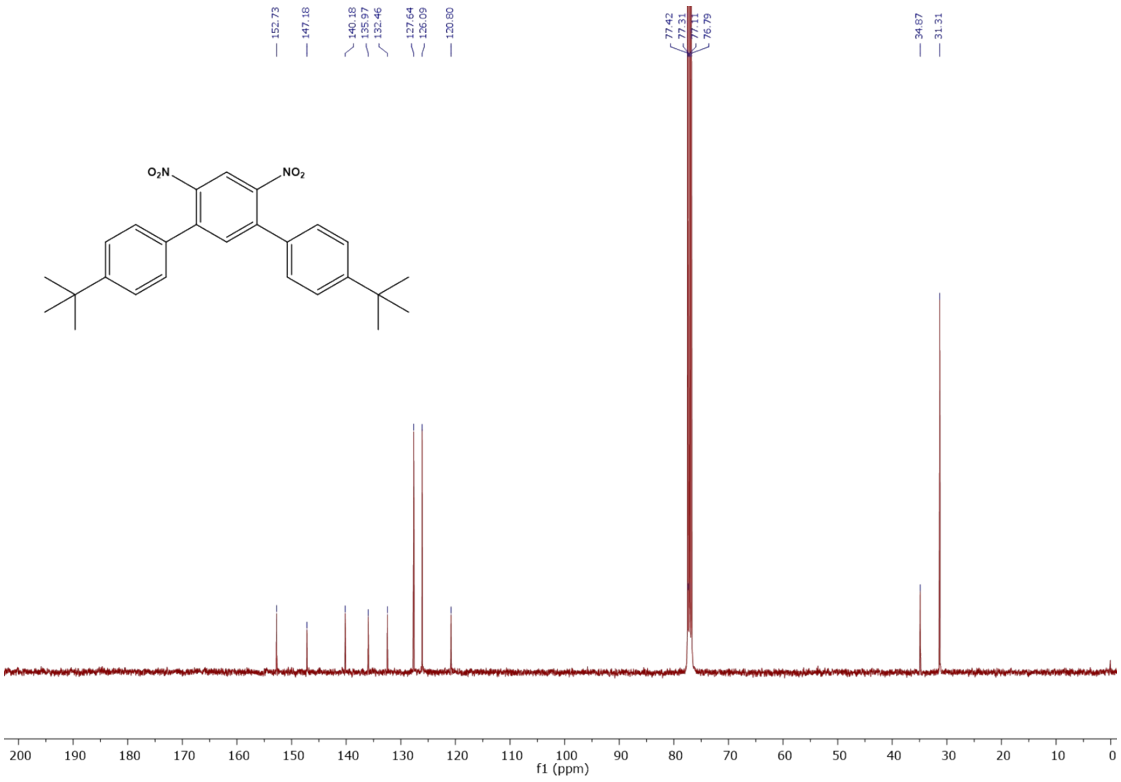

Figure S15. ^{13}C NMR spectra of compound (3) in $CDCl_3$.

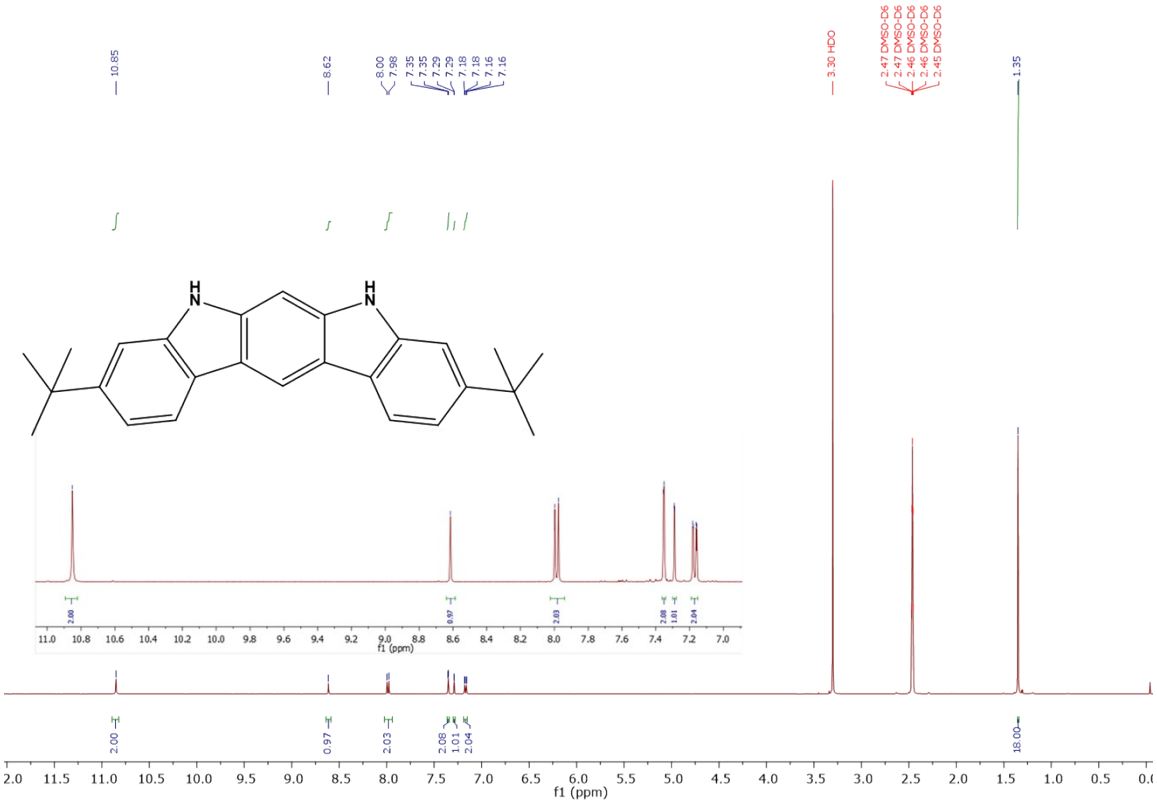

Figure S16. [1]H NMR spectra of compound (4) in DMSO.

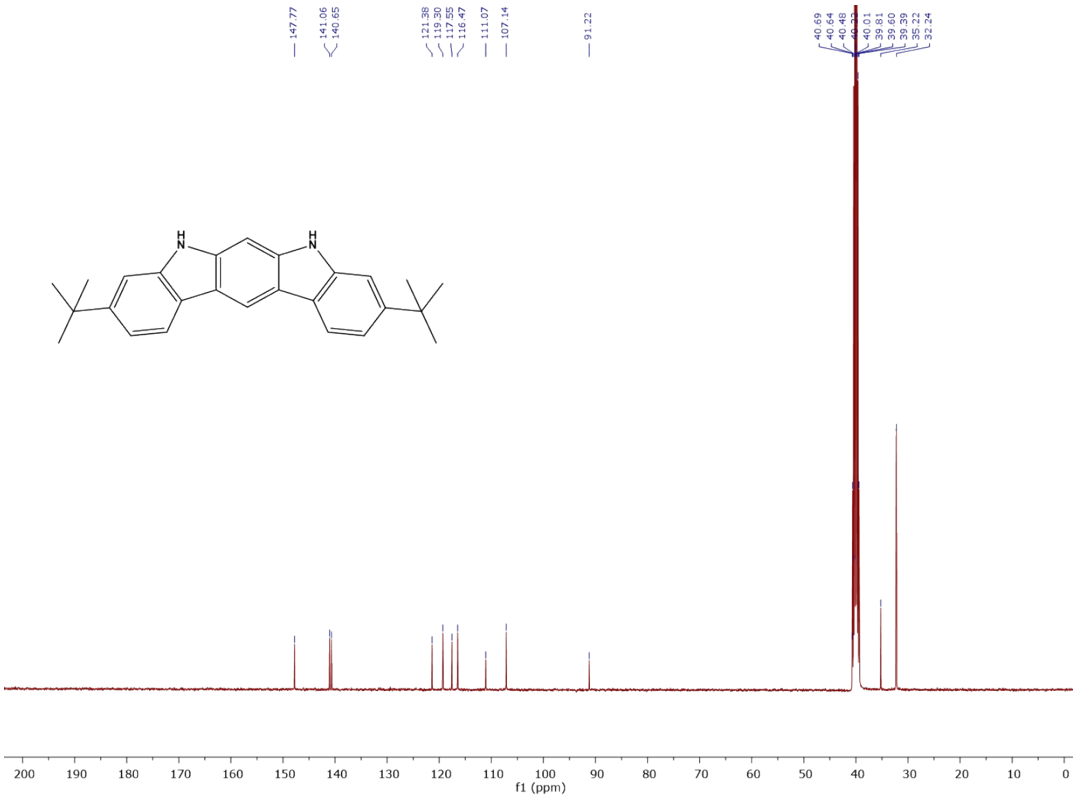

Figure S17. [13]C NMR spectra of compound (4) in DMSO.

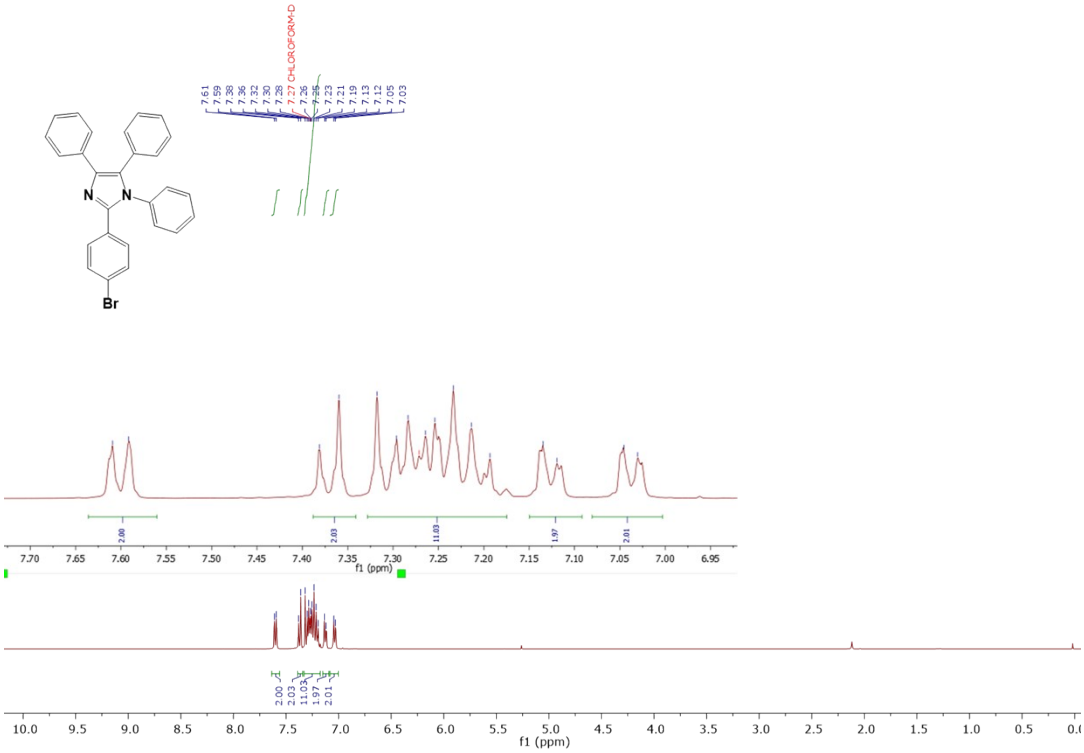

Figure S18. ^{1}H NMR spectra of compound (5) in $CDCl_3$.

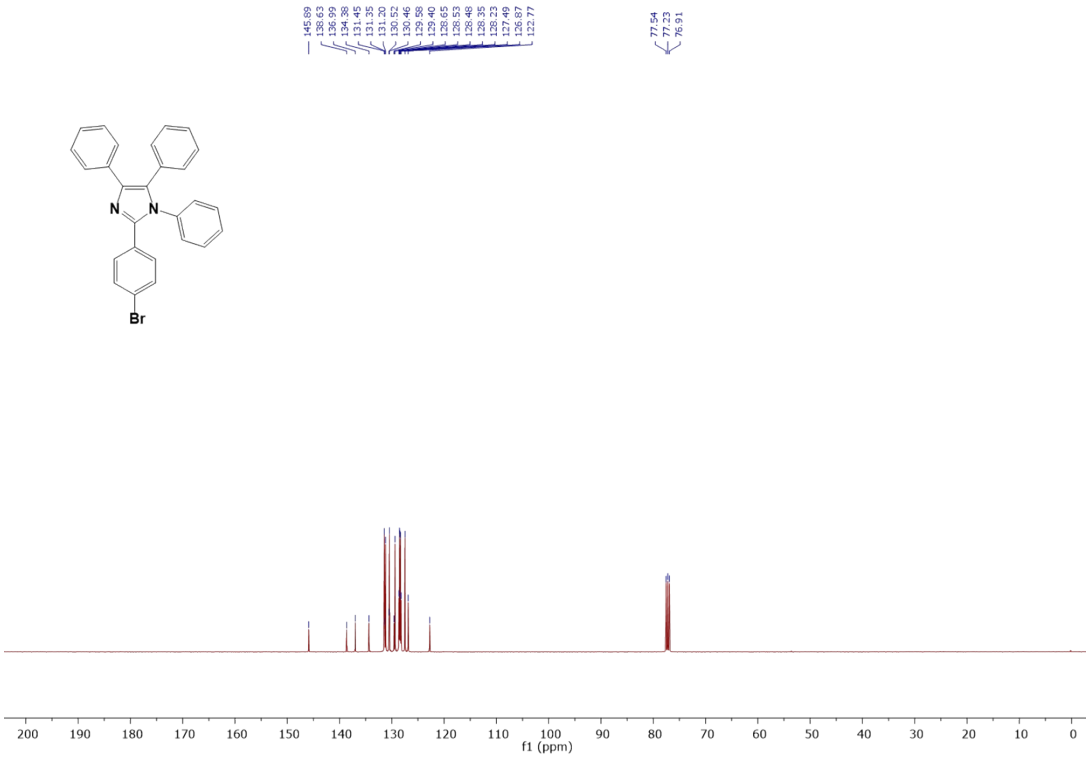

Figure S19. ^{13}C NMR spectra of compound (5) in $CDCl_3$.

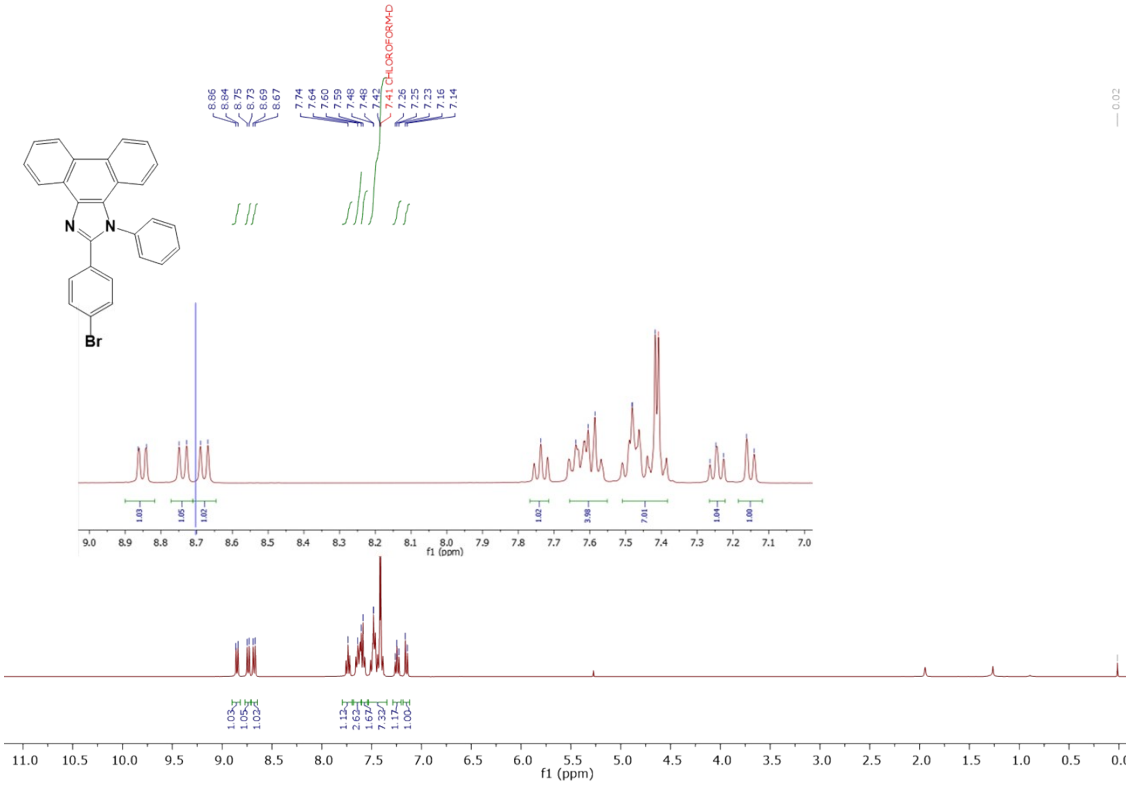

Figure S20. ^{1}H NMR spectra of compound (6) in $CDCl_3$.

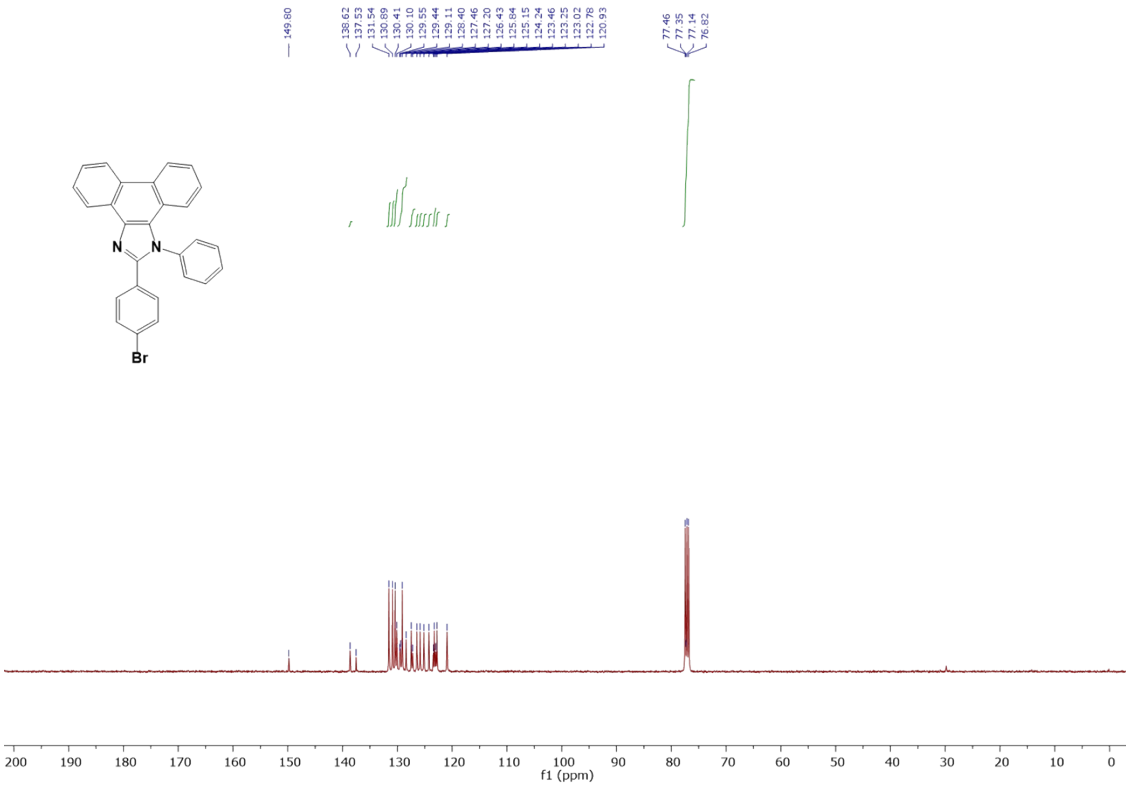

Figure S21. ^{13}C NMR spectra of compound (6) in $CDCl_3$.

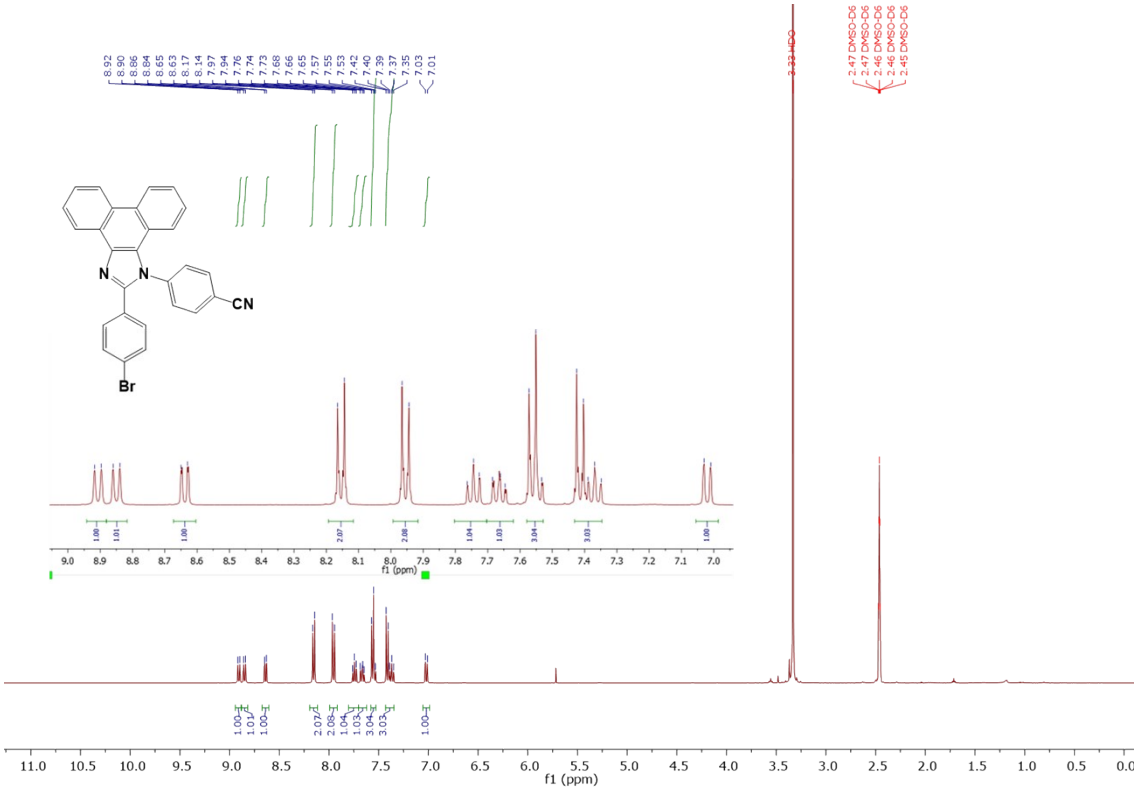

Figure S22. [1]H NMR spectra of compound (7) in DMSO.

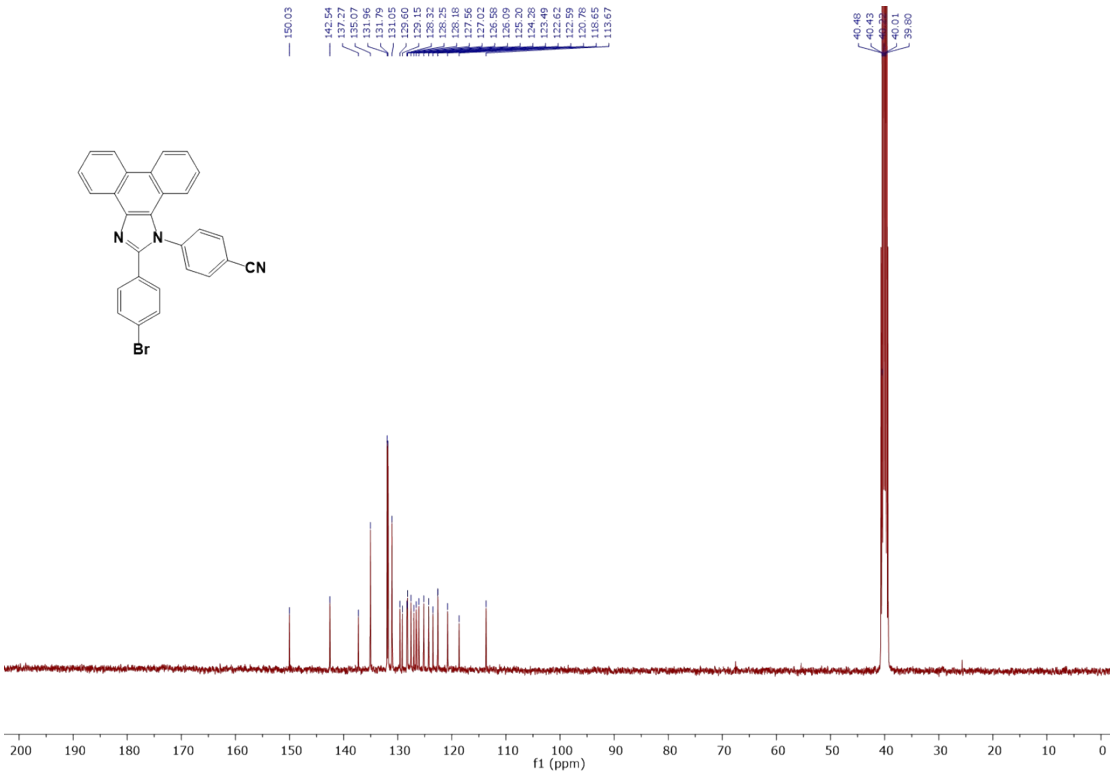

Figure S23. [13]C NMR spectra of compound (7) in DMSO.

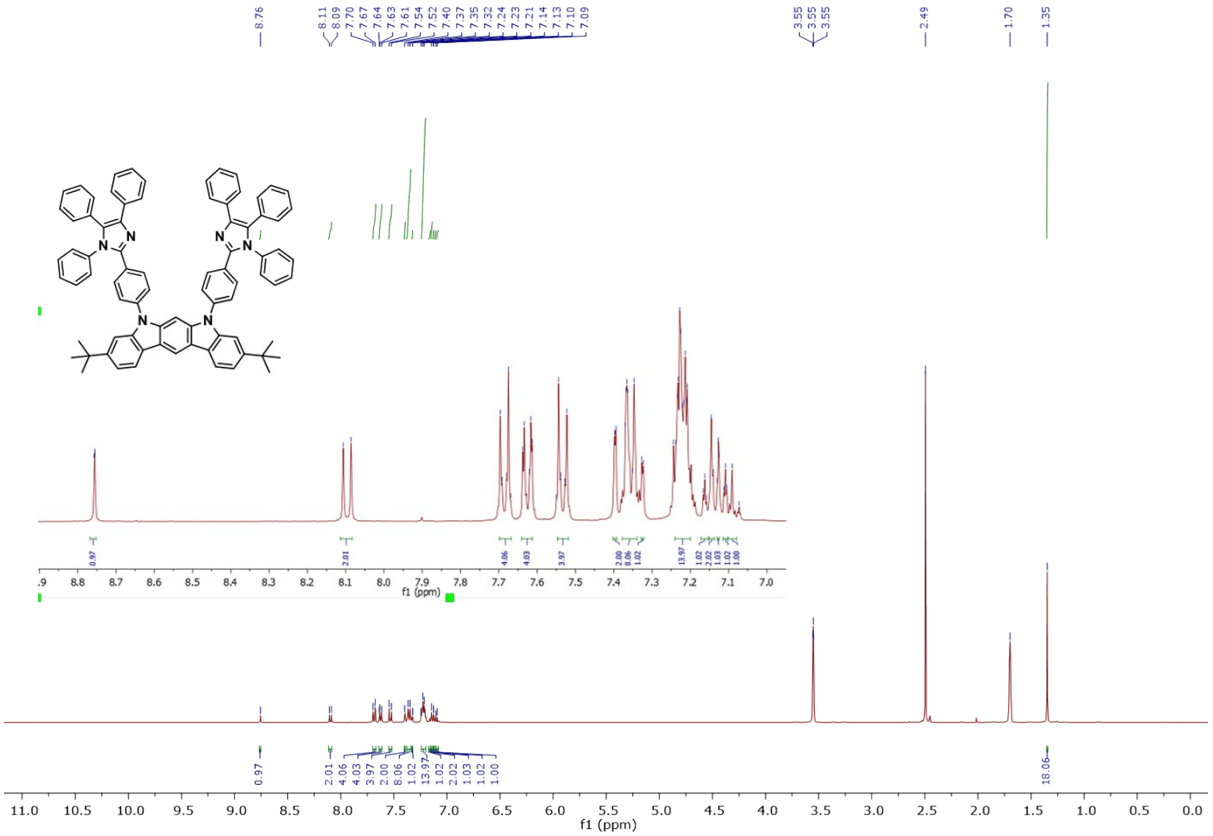

Figure S24. ^{1}H NMR spectra of TPI-InCz in THF

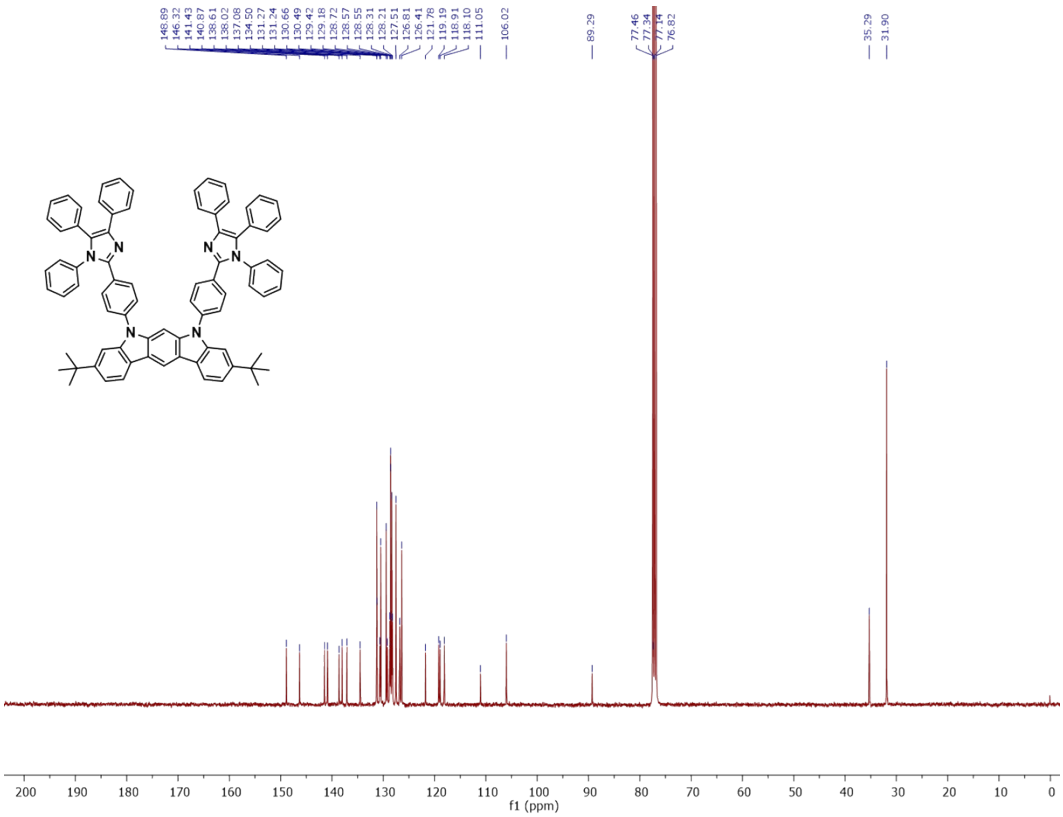

Figure S25. ^{13}C NMR spectra of TPI-InCz in $CDCl_3$.

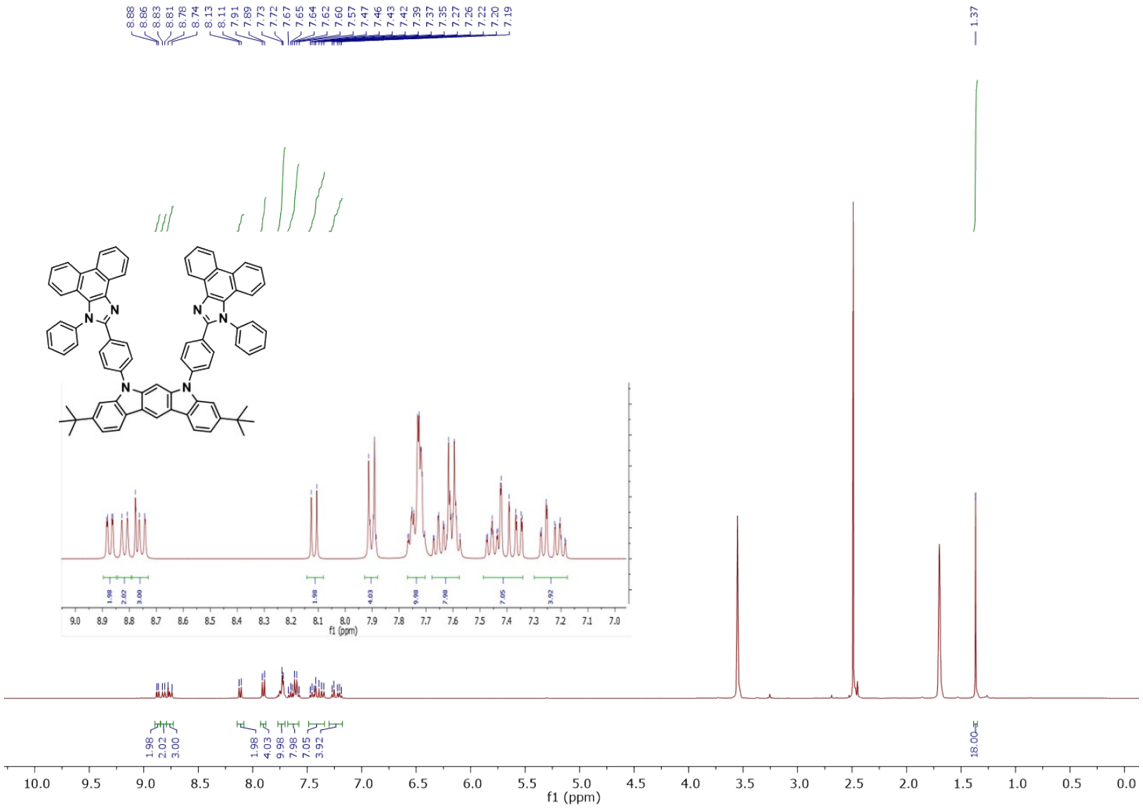

Figure S26. ^{1}H NMR spectra of PAI-InCz in THF.

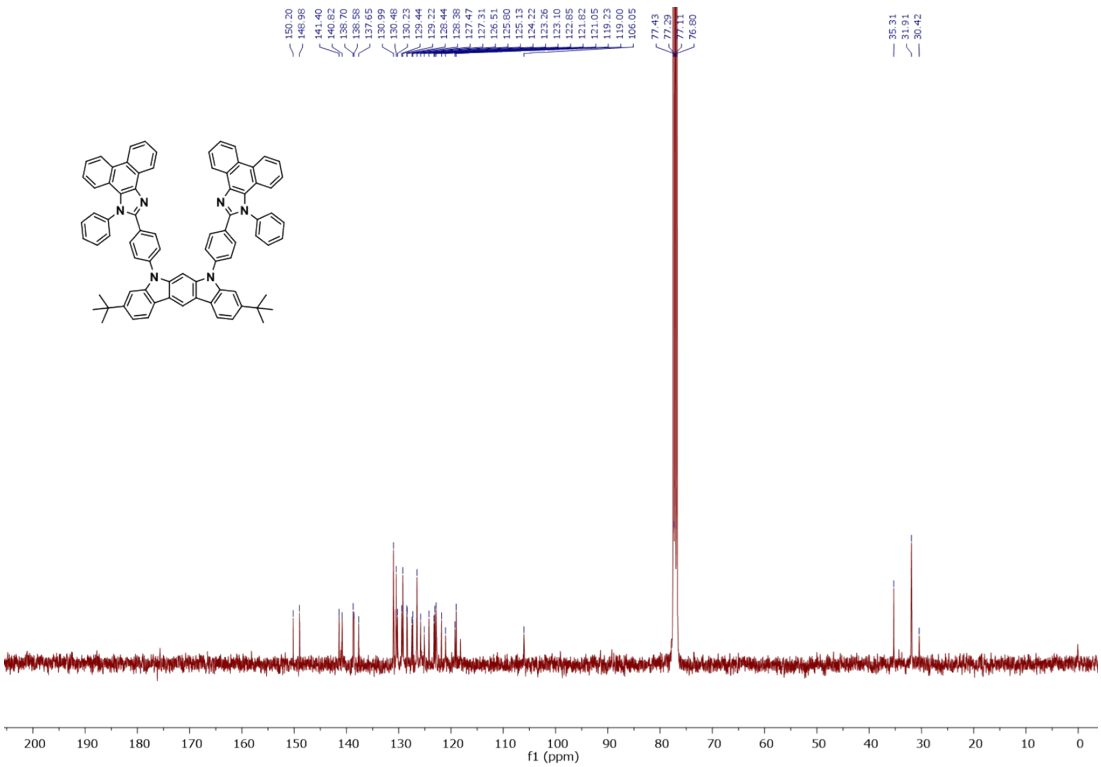

Figure S27. ^{13}C NMR spectra of PAI-InCz in $CDCl_3$.

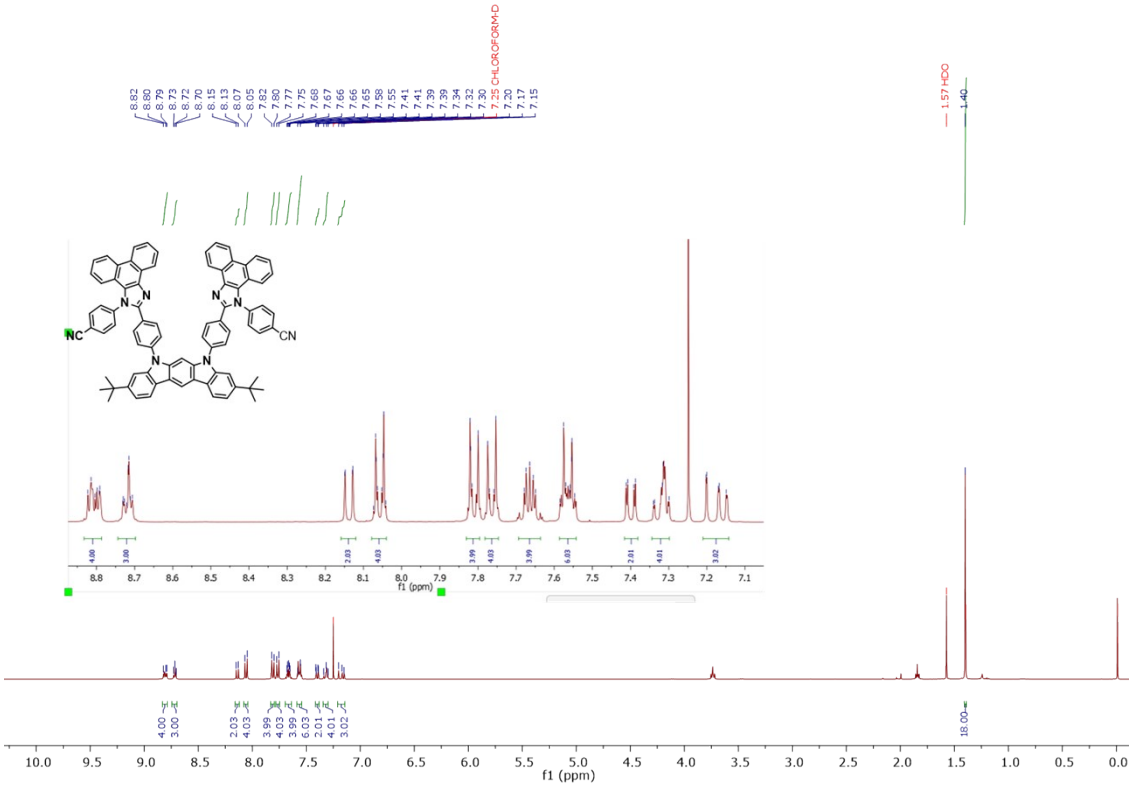

Figure S28. ^{1}H NMR spectra of CN-PAI-InCz in $CDCl_3$.

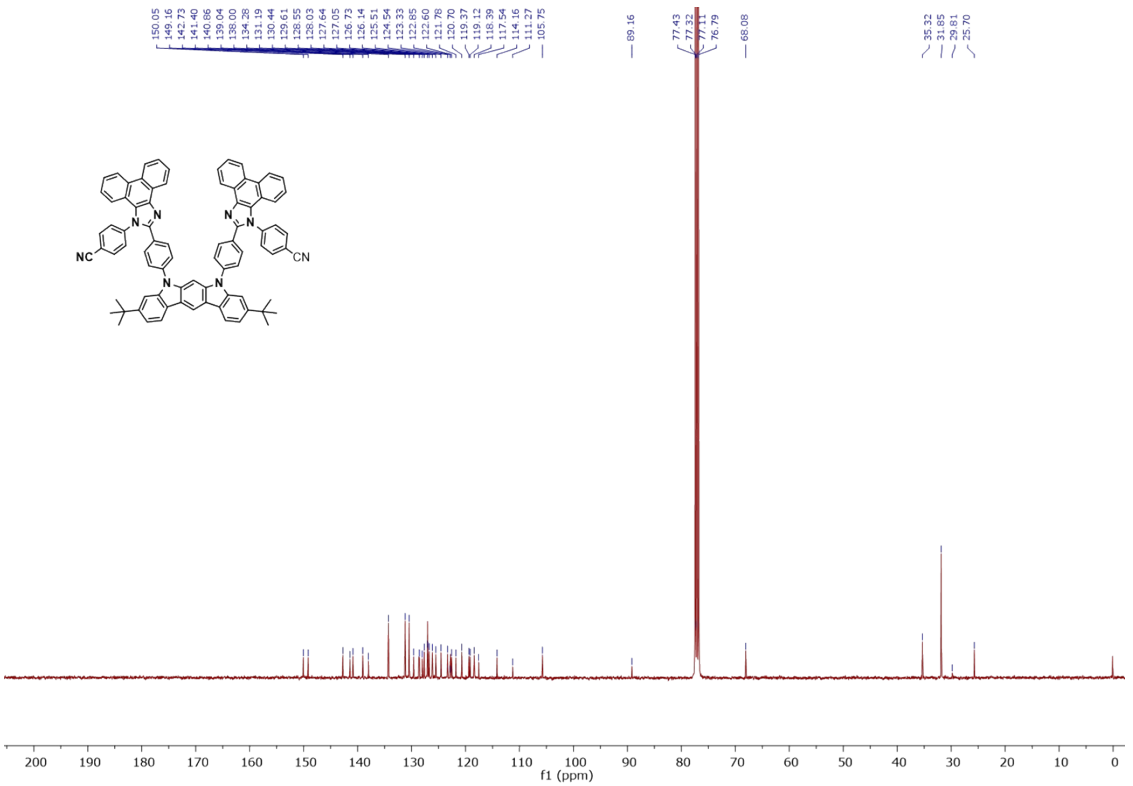

Figure S29. ^{13}C NMR spectra of CN-PAI-InCz in $CDCl_3$.

Table S3. Crystal data and structure refinement for CN-PAI-InCz.

Identification code	CN-PAI-InCz	
Empirical formula	C86 H66 N8 O	
Formula weight	1227.46	
Temperature	98(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.8165(2) Å	α= 90°.
	b = 31.2237(6) Å	β= 102.2250(10)°.
	c = 16.4633(3) Å	γ = 90°.
Volume	6438.9(2) $Å^3$	
Z	4	
Density (calculated)	1.266 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	2584	
Crystal size	0.253 x 0.122 x 0.083 mm^3	
Theta range for data collection	1.626 to 27.595°.	
Index ranges	-16<=h<=16, -40<=k<=40, -21<=l<=21	
Reflections collected	178316	
Independent reflections	14836 [R(int) = 0.0708]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.7107	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14836 / 0 / 856	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.1028	
R indices (all data)	R1 = 0.0716, wR2 = 0.1147	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.376 and -0.459 $e.Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for CN-PAI-InCz.

N(1)-C(12)	1.4006(19)	C(7)-C(12)	1.421(2)	C(23)-C(26)	1.531(2)	C(38)-C(39)	1.396(3)
N(1)-C(1)	1.4078(18)	C(8)-C(9)	1.390(2)	C(23)-C(25)	1.536(2)	C(38)-H(38A)	0.95
N(1)-C(27)	1.4152(18)	C(8)-H(8A)	0.95	C(23)-C(24)	1.537(2)	C(39)-C(40)	1.368(3)
N(2)-C(10)	1.3973(19)	C(9)-C(10)	1.418(2)	C(24)-H(24A)	0.98	C(39)-H(39A)	0.95
N(2)-C(13)	1.3993(19)	C(9)-C(14)	1.451(2)	C(24)-H(24B)	0.98	C(40)-C(41)	1.412(2)
N(2)-C(55)	1.4190(18)	C(10)-C(11)	1.388(2)	C(24)-H(24C)	0.98	C(40)-H(40A)	0.95
N(3)-C(33)	1.3132(19)	C(11)-C(12)	1.388(2)	C(25)-H(25A)	0.98	C(41)-C(42)	1.464(2)
N(3)-C(34)	1.3832(19)	C(11)-H(11A)	0.95	C(25)-H(25B)	0.98	C(42)-C(43)	1.405(2)
N(4)-C(33)	1.3862(19)	C(13)-C(18)	1.391(2)	C(25)-H(25C)	0.98	C(42)-C(47)	1.423(2)
N(4)-C(35)	1.3890(19)	C(13)-C(14)	1.404(2)	C(26)-H(26A)	0.98	C(43)-C(44)	1.372(2)
N(4)-C(48)	1.4309(19)	C(14)-C(15)	1.394(2)	C(26)-H(26B)	0.98	C(43)-H(43A)	0.95
N(5)-C(54)	1.145(2)	C(15)-C(16)	1.385(2)	C(26)-H(26C)	0.98	C(44)-C(45)	1.394(2)
N(6)-C(61)	1.3141(19)	C(15)-H(15A)	0.95	C(27)-C(32)	1.389(2)	C(44)-H(44A)	0.95
N(6)-C(62)	1.3739(19)	C(16)-C(17)	1.405(2)	C(27)-C(28)	1.392(2)	C(45)-C(46)	1.370(2)
N(7)-C(61)	1.3823(19)	C(16)-H(16A)	0.95	C(33)-C(30)	1.469(2)	C(45)-H(45A)	0.95
N(7)-C(63)	1.3899(19)	C(17)-C(18)	1.390(2)	C(34)-C(35)	1.372(2)	C(46)-C(47)	1.407(2)
N(7)-C(76)	1.4272(19)	C(17)-C(23)	1.535(2)	C(34)-C(36)	1.432(2)	C(46)-H(46A)	0.95
N(8)-C(82)	1.147(2)	C(18)-H(18A)	0.95	C(28)-C(29)	1.379(2)	C(48)-C(49)	1.383(2)
C(1)-C(2)	1.387(2)	C(19)-C(22)	1.527(2)	C(28)-H(28A)	0.95	C(48)-C(53)	1.389(2)
C(1)-C(6)	1.402(2)	C(19)-C(20)	1.533(2)	C(35)-C(47)	1.429(2)	C(49)-C(50)	1.384(2)
C(2)-C(3)	1.394(2)	C(19)-C(21)	1.538(2)	C(29)-C(30)	1.395(2)	C(49)-H(49A)	0.95
C(2)-H(2A)	0.95	C(20)-H(20A)	0.98	C(29)-H(29A)	0.95	C(50)-C(51)	1.395(2)
C(3)-C(4)	1.400(2)	C(20)-H(20B)	0.98	C(30)-C(31)	1.401(2)	C(50)-H(50A)	0.95
C(3)-C(19)	1.537(2)	C(20)-H(20C)	0.98	C(36)-C(37)	1.402(2)	C(51)-C(52)	1.395(2)
C(4)-C(5)	1.387(2)	C(21)-H(21A)	0.98	C(36)-C(41)	1.420(2)	C(51)-C(54)	1.442(2)
C(4)-H(4A)	0.95	C(21)-H(21B)	0.98	C(31)-C(32)	1.389(2)	C(52)-C(53)	1.374(2)
C(5)-C(6)	1.394(2)	C(21)-H(21C)	0.98	C(31)-H(31A)	0.95	C(52)-H(52A)	0.95
C(5)-H(5A)	0.95	C(22)-H(22A)	0.98	C(37)-C(38)	1.376(2)	C(53)-H(53A)	0.95
C(6)-C(7)	1.447(2)	C(22)-H(22B)	0.98	C(37)-H(37A)	0.95	C(55)-C(60)	1.388(2)
C(7)-C(8)	1.391(2)	C(22)-H(22C)	0.98	C(32)-H(32A)	0.95	C(55)-C(56)	1.393(2)

C(12)-N(1)-C(1)	108.32(12)	C(8)-C(7)-C(6)	133.25(14)
C(12)-N(1)-C(27)	126.12(12)	C(12)-C(7)-C(6)	106.82(13)
C(1)-N(1)-C(27)	125.31(12)	C(9)-C(8)-C(7)	118.50(13)
C(10)-N(2)-C(13)	108.54(12)	C(9)-C(8)-H(8A)	120.7
C(10)-N(2)-C(55)	125.43(12)	C(7)-C(8)-H(8A)	120.7
C(13)-N(2)-C(55)	125.74(12)	C(8)-C(9)-C(10)	119.82(13)
C(33)-N(3)-C(34)	105.06(12)	C(8)-C(9)-C(14)	133.86(14)
C(33)-N(4)-C(35)	106.06(12)	C(10)-C(9)-C(14)	106.32(12)
C(33)-N(4)-C(48)	124.05(12)	C(11)-C(10)-N(2)	127.81(13)
C(35)-N(4)-C(48)	127.25(12)	C(11)-C(10)-C(9)	123.26(13)
C(61)-N(6)-C(62)	105.60(12)	N(2)-C(10)-C(9)	108.88(13)
C(61)-N(7)-C(63)	106.53(12)	C(10)-C(11)-C(12)	115.48(13)
C(61)-N(7)-C(76)	127.11(12)	C(10)-C(11)-H(11A)	122.3
C(63)-N(7)-C(76)	126.33(12)	C(12)-C(11)-H(11A)	122.3
C(2)-C(1)-C(6)	122.25(13)	C(11)-C(12)-N(1)	128.39(13)
C(2)-C(1)-N(1)	128.77(14)	C(11)-C(12)-C(7)	122.97(14)
C(6)-C(1)-N(1)	108.91(13)	N(1)-C(12)-C(7)	108.56(12)
C(1)-C(2)-C(3)	119.26(14)	C(18)-C(13)-N(2)	128.75(14)
C(1)-C(2)-H(2A)	120.4	C(18)-C(13)-C(14)	122.43(14)
C(3)-C(2)-H(2A)	120.4	N(2)-C(13)-C(14)	108.81(13)
C(2)-C(3)-C(4)	118.59(14)	C(15)-C(14)-C(13)	118.19(14)
C(2)-C(3)-C(19)	118.73(14)	C(15)-C(14)-C(9)	134.37(14)
C(4)-C(3)-C(19)	122.67(14)	C(13)-C(14)-C(9)	107.43(13)
C(5)-C(4)-C(3)	121.93(14)	C(16)-C(15)-C(14)	119.48(14)
C(5)-C(4)-H(4A)	119	C(16)-C(15)-H(15A)	120.3
C(3)-C(4)-H(4A)	119	C(14)-C(15)-H(15A)	120.3
C(4)-C(5)-C(6)	119.66(14)	C(15)-C(16)-C(17)	122.18(14)
C(4)-C(5)-H(5A)	120.2	C(15)-C(16)-H(16A)	118.9
C(6)-C(5)-H(5A)	120.2	C(17)-C(16)-H(16A)	118.9
C(5)-C(6)-C(1)	118.18(14)	C(18)-C(17)-C(16)	118.60(14)
C(5)-C(6)-C(7)	134.45(14)	C(18)-C(17)-C(23)	120.53(14)
C(1)-C(6)-C(7)	107.37(13)	C(16)-C(17)-C(23)	120.68(14)
C(8)-C(7)-C(12)	119.92(13)	C(17)-C(18)-C(13)	119.08(14)

C(17)-C(18)-H(18A)	120.5	C(23)-C(24)-H(24B)	109.5
C(13)-C(18)-H(18A)	120.5	H(24A)-C(24)-H(24B)	109.5
C(22)-C(19)-C(20)	107.61(13)	C(23)-C(24)-H(24C)	109.5
C(22)-C(19)-C(3)	112.22(13)	H(24A)-C(24)-H(24C)	109.5
C(20)-C(19)-C(3)	110.10(13)	H(24B)-C(24)-H(24C)	109.5
C(22)-C(19)-C(21)	108.70(13)	C(23)-C(25)-H(25A)	109.5
C(20)-C(19)-C(21)	108.90(14)	C(23)-C(25)-H(25B)	109.5
C(3)-C(19)-C(21)	109.23(13)	H(25A)-C(25)-H(25B)	109.5
C(19)-C(20)-H(20A)	109.5	C(23)-C(25)-H(25C)	109.5
C(19)-C(20)-H(20B)	109.5	H(25A)-C(25)-H(25C)	109.5
H(20A)-C(20)-H(20B)	109.5	H(25B)-C(25)-H(25C)	109.5
C(19)-C(20)-H(20C)	109.5	C(23)-C(26)-H(26A)	109.5
H(20A)-C(20)-H(20C)	109.5	C(23)-C(26)-H(26B)	109.5
H(20B)-C(20)-H(20C)	109.5	H(26A)-C(26)-H(26B)	109.5
C(19)-C(21)-H(21A)	109.5	C(23)-C(26)-H(26C)	109.5
C(19)-C(21)-H(21B)	109.5	H(26A)-C(26)-H(26C)	109.5
H(21A)-C(21)-H(21B)	109.5	H(26B)-C(26)-H(26C)	109.5
C(19)-C(21)-H(21C)	109.5	C(32)-C(27)-C(28)	119.39(13)
H(21A)-C(21)-H(21C)	109.5	C(32)-C(27)-N(1)	120.35(13)
H(21B)-C(21)-H(21C)	109.5	C(28)-C(27)-N(1)	120.26(13)
C(19)-C(22)-H(22A)	109.5	N(3)-C(33)-N(4)	112.25(13)
C(19)-C(22)-H(22B)	109.5	N(3)-C(33)-C(30)	122.80(13)
H(22A)-C(22)-H(22B)	109.5	N(4)-C(33)-C(30)	124.91(13)
C(19)-C(22)-H(22C)	109.5	C(35)-C(34)-N(3)	111.04(13)
H(22A)-C(22)-H(22C)	109.5	C(35)-C(34)-C(36)	121.63(14)
H(22B)-C(22)-H(22C)	109.5	N(3)-C(34)-C(36)	127.09(14)
C(26)-C(23)-C(17)	111.73(13)	C(29)-C(28)-C(27)	120.46(14)
C(26)-C(23)-C(25)	108.49(14)	C(29)-C(28)-H(28A)	119.8
C(17)-C(23)-C(25)	108.02(13)	C(27)-C(28)-H(28A)	119.8
C(26)-C(23)-C(24)	108.29(13)	C(34)-C(35)-N(4)	105.55(13)
C(17)-C(23)-C(24)	112.08(13)	C(34)-C(35)-C(47)	123.62(14)
C(25)-C(23)-C(24)	108.11(14)	N(4)-C(35)-C(47)	130.81(14)
C(23)-C(24)-H(24A)	109.5	C(28)-C(29)-C(30)	121.07(14)

C(28)-C(29)-H(29A)	119.5	C(44)-C(43)-H(43A)	119
C(30)-C(29)-H(29A)	119.5	C(42)-C(43)-H(43A)	119
C(29)-C(30)-C(31)	118.11(13)	C(43)-C(44)-C(45)	120.26(16)
C(29)-C(30)-C(33)	117.94(13)	C(43)-C(44)-H(44A)	119.9
C(31)-C(30)-C(33)	123.75(13)	C(45)-C(44)-H(44A)	119.9
C(37)-C(36)-C(41)	120.61(14)	C(46)-C(45)-C(44)	119.83(16)
C(37)-C(36)-C(34)	122.30(15)	C(46)-C(45)-H(45A)	120.1
C(41)-C(36)-C(34)	117.05(14)	C(44)-C(45)-H(45A)	120.1
C(32)-C(31)-C(30)	120.95(14)	C(45)-C(46)-C(47)	120.71(16)
C(32)-C(31)-H(31A)	119.5	C(45)-C(46)-H(46A)	119.6
C(30)-C(31)-H(31A)	119.5	C(47)-C(46)-H(46A)	119.6
C(38)-C(37)-C(36)	120.51(16)	C(46)-C(47)-C(42)	119.89(14)
C(38)-C(37)-H(37A)	119.7	C(46)-C(47)-C(35)	124.28(14)
C(36)-C(37)-H(37A)	119.7	C(42)-C(47)-C(35)	115.83(14)
C(27)-C(32)-C(31)	120.01(13)	C(49)-C(48)-C(53)	121.31(14)
C(27)-C(32)-H(32A)	120	C(49)-C(48)-N(4)	119.99(13)
C(31)-C(32)-H(32A)	120	C(53)-C(48)-N(4)	118.48(13)
C(37)-C(38)-C(39)	119.50(17)	C(48)-C(49)-C(50)	119.23(14)
C(37)-C(38)-H(38A)	120.2	C(48)-C(49)-H(49A)	120.4
C(39)-C(38)-H(38A)	120.2	C(50)-C(49)-H(49A)	120.4
C(40)-C(39)-C(38)	120.79(16)	C(49)-C(50)-C(51)	119.58(15)
C(40)-C(39)-H(39A)	119.6	C(49)-C(50)-H(50A)	120.2
C(38)-C(39)-H(39A)	119.6	C(51)-C(50)-H(50A)	120.2
C(39)-C(40)-C(41)	121.67(17)	C(52)-C(51)-C(50)	120.65(14)
C(39)-C(40)-H(40A)	119.2	C(52)-C(51)-C(54)	118.26(14)
C(41)-C(40)-H(40A)	119.2	C(50)-C(51)-C(54)	121.08(14)
C(40)-C(41)-C(36)	116.93(15)	C(53)-C(52)-C(51)	119.43(14)
C(40)-C(41)-C(42)	122.50(15)	C(53)-C(52)-H(52A)	120.3
C(36)-C(41)-C(42)	120.57(14)	C(51)-C(52)-H(52A)	120.3
C(43)-C(42)-C(47)	117.13(15)	C(52)-C(53)-C(48)	119.68(14)
C(43)-C(42)-C(41)	122.03(15)	C(52)-C(53)-H(53A)	120.2
C(47)-C(42)-C(41)	120.84(14)	C(48)-C(53)-H(53A)	120.2
C(44)-C(43)-C(42)	121.94(16)	N(5)-C(54)-C(51)	177.44(18)

C(60)-C(55)-C(56)	119.62(13)	C(65)-C(66)-C(67)	119.53(18)
C(60)-C(55)-N(2)	120.64(13)	C(65)-C(66)-H(66A)	120.2
C(56)-C(55)-N(2)	119.74(13)	C(67)-C(66)-H(66A)	120.2
C(57)-C(56)-C(55)	120.10(14)	C(68)-C(67)-C(66)	120.65(17)
C(57)-C(56)-H(56A)	119.9	C(68)-C(67)-H(67A)	119.7
C(55)-C(56)-H(56A)	119.9	C(66)-C(67)-H(67A)	119.7
C(56)-C(57)-C(58)	121.13(14)	C(67)-C(68)-C(69)	121.70(17)
C(56)-C(57)-H(57A)	119.4	C(67)-C(68)-H(68A)	119.2
C(58)-C(57)-H(57A)	119.4	C(69)-C(68)-H(68A)	119.2
C(57)-C(58)-C(59)	118.18(13)	C(68)-C(69)-C(64)	117.04(16)
C(57)-C(58)-C(61)	117.01(13)	C(68)-C(69)-C(70)	122.33(16)
C(59)-C(58)-C(61)	124.68(13)	C(64)-C(69)-C(70)	120.60(14)
C(60)-C(59)-C(58)	120.96(14)	C(71)-C(70)-C(75)	117.61(16)
C(60)-C(59)-H(59A)	119.5	C(71)-C(70)-C(69)	120.99(15)
C(58)-C(59)-H(59A)	119.5	C(75)-C(70)-C(69)	121.38(14)
C(59)-C(60)-C(55)	119.99(14)	C(72)-C(71)-C(70)	122.03(16)
C(59)-C(60)-H(60A)	120	C(72)-C(71)-H(71A)	119
C(55)-C(60)-H(60A)	120	C(70)-C(71)-H(71A)	119
N(6)-C(61)-N(7)	111.64(13)	C(71)-C(72)-C(73)	120.24(16)
N(6)-C(61)-C(58)	122.30(13)	C(71)-C(72)-H(72A)	119.9
N(7)-C(61)-C(58)	125.96(13)	C(73)-C(72)-H(72A)	119.9
C(63)-C(62)-N(6)	111.08(13)	C(74)-C(73)-C(72)	119.68(18)
C(63)-C(62)-C(64)	121.76(14)	C(74)-C(73)-H(73A)	120.2
N(6)-C(62)-C(64)	127.07(14)	C(72)-C(73)-H(73A)	120.2
C(62)-C(63)-N(7)	105.12(13)	C(73)-C(74)-C(75)	121.17(16)
C(62)-C(63)-C(75)	123.30(14)	C(73)-C(74)-H(74A)	119.4
N(7)-C(63)-C(75)	131.55(14)	C(75)-C(74)-H(74A)	119.4
C(65)-C(64)-C(69)	120.67(15)	C(74)-C(75)-C(70)	119.25(14)
C(65)-C(64)-C(62)	122.28(15)	C(74)-C(75)-C(63)	125.17(14)
C(69)-C(64)-C(62)	117.02(14)	C(70)-C(75)-C(63)	115.58(14)
C(66)-C(65)-C(64)	120.37(17)	C(77)-C(76)-C(81)	121.34(14)
C(66)-C(65)-H(65A)	119.8	C(77)-C(76)-N(7)	119.43(14)
C(64)-C(65)-H(65A)	119.8	C(81)-C(76)-N(7)	119.22(14)

C(76)-C(77)-C(78)	119.45(15)	O(1)-C(83)-H(83B)	110.6
C(76)-C(77)-H(77A)	120.3	C(84)-C(83)-H(83B)	110.6
C(78)-C(77)-H(77A)	120.3	H(83A)-C(83)-H(83B)	108.8
C(77)-C(78)-C(79)	119.57(15)	C(83)-C(84)-C(85)	102.25(15)
C(77)-C(78)-H(78A)	120.2	C(83)-C(84)-H(84A)	111.3
C(79)-C(78)-H(78A)	120.2	C(85)-C(84)-H(84A)	111.3
C(80)-C(79)-C(78)	120.82(15)	C(83)-C(84)-H(84B)	111.3
C(80)-C(79)-C(82)	120.46(15)	C(85)-C(84)-H(84B)	111.3
C(78)-C(79)-C(82)	118.69(15)	H(84A)-C(84)-H(84B)	109.2
C(81)-C(80)-C(79)	119.34(15)	C(86)-C(85)-C(84)	103.02(17)
C(81)-C(80)-H(80A)	120.3	C(86)-C(85)-H(85A)	111.2
C(79)-C(80)-H(80A)	120.3	C(84)-C(85)-H(85A)	111.2
C(80)-C(81)-C(76)	119.47(15)	C(86)-C(85)-H(85B)	111.2
C(80)-C(81)-H(81A)	120.3	C(84)-C(85)-H(85B)	111.2
C(76)-C(81)-H(81A)	120.3	O(1)-C(86)-H(86A)	109.7
N(8)-C(82)-C(79)	176.43(19)	C(85)-C(86)-H(86A)	109.7
C(86)-O(1)-C(83)	108.10(17)	O(1)-C(86)-H(86B)	109.7
O(1)-C(83)-C(84)	105.57(15)	C(85)-C(86)-H(86B)	109.7
O(1)-C(83)-H(83A)	110.6	H(86A)-C(86)-H(86B)	108.2
C(84)-C(83)-H(83A)	110.6		

Symmetry transformations used to generate equivalent atoms:

Table S5. Geometry-optimized structures in Cartesian coordinates of TPI-InCz with B3LYP-D3/6-31G(d) by ORCA

H	-0.11340574698592	1.92167152233179	6.35452814200582
C	-0.54162026885812	2.66047120830854	5.68342719886732
C	-1.70862322030176	3.33814230716492	6.04247736898531
H	-2.19600450805830	3.12372490491611	6.98915200764564
C	-2.26325426138537	4.28274169167922	5.17836472955006
H	-3.19103978669306	4.78654167040827	5.42766551507851
C	-1.63748600686928	4.55866869016184	3.96190223888338
C	-0.47386240150127	3.87876092330971	3.59687195004454
H	-0.01240389342397	4.09369972311831	2.63945417545203
C	0.07019330827094	2.92771237215417	4.45771803821640
H	0.98385997884675	2.41073097334462	4.18271097297696
N	-2.21131124044373	5.49256587567513	3.03995540174387
C	-2.69069589679371	5.15597314648710	1.78161090935111
N	-2.87908579071737	6.23120698514085	1.04275073191618
C	-2.50830559708219	7.31479207549005	1.81330150042094
C	-2.06349519582298	6.88619726916505	3.05909202967938
C	-1.40049209997730	7.61776871803017	4.14850366831087
C	-1.81106200561932	7.51923213164170	5.48788082978080
H	-2.67394905759701	6.91463501280217	5.73994494662943
C	-1.13477253607271	8.21116547100234	6.49348809181730
H	-1.46703541142725	8.11918072616001	7.52405111349177
C	-0.04422677704989	9.02296674099449	6.17685857853669
H	0.48679352317261	9.55591625948339	6.96072407291287
C	0.36021160540764	9.14948658552765	4.84566046567572
H	1.21146362500932	9.76902692644485	4.58629721167823
C	-0.31217236292561	8.45564775163728	3.84318539634613
H	0.00565250401457	8.55418112802557	2.80968995268308
C	-2.61896999047889	8.68151522785979	1.28389801806711
C	-2.59152885806264	8.87983350283524	-0.10674268735384
H	-2.50030030601530	8.01250243037052	-0.75202064064471
C	-2.68453539202703	10.16199879834421	-0.64323927775371
H	-2.65688171837888	10.29685087663609	-1.72137553525738
C	-2.81138707575515	11.27028855793526	0.19760491329782
H	-2.88252658666760	12.27046677154962	-0.22124922360271
C	-2.85654599745585	11.08192246054854	1.58086437132133
H	-2.97254715544777	11.93554744076558	2.24361340920839
C	-2.76705244436360	9.80041269076982	2.12079972129477
H	-2.82337016146872	9.66491080905129	3.19538743371343
C	-2.82745538366563	3.76701203058676	1.32727646679418
C	-3.32624913945767	2.74592196750921	2.15241500903198
H	-3.72283898815083	2.98813095679600	3.13196644908359
C	-3.26321526206521	1.41564401352921	1.75019685843924
H	-3.59424972714987	0.62092013513640	2.41122897932941
C	-2.70973860085444	1.09024658727434	0.50749554986657
C	-2.29861365660743	2.10820660970491	-0.36067671028552
H	-1.89408789984470	1.84280204868186	-1.33226132569426
C	-2.35425379177184	3.43628943677613	0.04784907810297
H	-1.99761893578948	4.23093738822831	-0.59895583450000
N	-2.44028296845424	-0.25952159814560	0.16850169139966
C	-1.13866274901180	-0.76454741650819	0.09812349272306
C	0.05321551282323	-0.05658429994804	0.22008924900158
H	0.07145754929643	1.01709699072869	0.35210394375603
C	1.21321301158283	-0.82430514745042	0.16603024589682
C	1.19937053086865	-2.23756650990533	-0.04096121090050
C	-0.01603362262434	-2.91860140329668	-0.14892361168342

H	-0.03861399478789	-3.99612769322140	-0.28769982219028
C	-1.20014079040046	-2.18174881151456	-0.06178675834214
C	-2.61008171665985	-2.53058137879695	-0.05857937936315
C	-3.32359922644304	-3.72820190790318	-0.16544580503742
H	-2.80030138350243	-4.67207915523170	-0.29479624862472
C	-4.71306320704272	-3.70239638749927	-0.10082698291602
H	-5.25267546893779	-4.64107457011724	-0.18015080753173
C	-5.43972142480133	-2.50083564820011	0.06549889305196
C	-4.73350318309121	-1.29721160502949	0.16630513515760
H	-5.24272238810084	-0.34901575835166	0.28696524595076
C	-3.34081382435734	-1.32766879539261	0.10705269066232
C	-6.97285587533683	-2.55311779849192	0.13632891595956
C	-7.39781040558108	-3.41098224748480	1.34926947914841
H	-8.49165565568922	-3.46082364745233	1.41802655598822
H	-7.01854263600686	-4.43509467578610	1.27378836981018
H	-7.01499051633809	-2.98029574927154	2.28157801794235
C	-7.52945778814535	-3.18489796852133	-1.15895475707628
H	-8.62463544359250	-3.23373449269036	-1.11878445691624
H	-7.24481110903317	-2.59049463591100	-2.03435976821235
H	-7.15397461558153	-4.20216341313921	-1.30928234905675
C	-7.59879254265664	-1.15678730801314	0.29435504312137
H	-8.69022364918948	-1.24432699516928	0.33653350057752
H	-7.34910877582177	-0.50338302772441	-0.54913149316080
H	-7.26863250252403	-0.66750720715636	1.21769202997577
C	2.58755721153069	-2.65705082408642	-0.09192875533989
C	3.38559735378647	-1.50132914321130	0.08902760839271
C	4.77907376625638	-1.55747016552238	0.12228252560677
H	5.35045303258261	-0.65339420183477	0.28604885639422
C	5.41252026374774	-2.79280722969861	-0.05163594743363
C	4.61613106859812	-3.94485397826472	-0.24068448256287
H	5.09871300720206	-4.90799010979006	-0.37486508858258
C	3.22655357970454	-3.88919574380073	-0.25811797694385
H	2.64460515828600	-4.79650664378783	-0.39792221897708
C	6.94194923272447	-2.92986765253843	-0.03590449700449
C	7.64948640006900	-1.57332848083982	0.12423158818996
H	8.73538746813442	-1.71938763876355	0.10981695607308
H	7.39290491154075	-1.08989383118003	1.07366993707539
H	7.39452965057650	-0.88654602734332	-0.69090235422979
C	7.36063842420414	-3.83584976918071	1.14349516127867
H	8.45140521064770	-3.95094178464608	1.16978432947769
H	7.03797486590771	-3.40307104897784	2.09729444788197
H	6.91863722125972	-4.83421110366936	1.06297380883006
C	7.41763501230496	-3.56195980796906	-1.36315626850648
H	8.50944582295397	-3.66804372095263	-1.36428088833276
H	6.98502651788179	-4.55519333002908	-1.52030688800080
H	7.13356876569498	-2.93504225133229	-2.21585337535551
N	2.54189283921023	-0.39161572240977	0.25319762718146
C	2.93758544179077	0.94322120867054	0.49628466236427
C	3.88707849774230	1.57192064271368	-0.32106785277141
H	4.32891376754754	1.02135068226051	-1.14492184036112
C	4.23126467072901	2.89958743538676	-0.09912994014238
H	4.94382358332866	3.39908183320918	-0.74590950340453
C	3.62819458781873	3.64474216229893	0.93137891081712
C	2.68232448923063	3.00327014504192	1.74828736436046
H	2.19499211455710	3.54811637207455	2.54507405390752
C	2.35207616509427	1.66781634170394	1.54256826693722
H	1.62094557405886	1.18307778549563	2.18088588085563
C	3.95034273822305	5.07371074782933	1.01815906410868
N	4.41507548390474	5.76296828077863	-0.01125566577032

C	4.51506370786818	7.07531276371873	0.38653939912260
C	4.08492268272770	7.20435278886572	1.70230631017545
N	3.74480448291403	5.90813675046405	2.10604684520585
C	3.32115795950030	5.55442782372093	3.42360575599334
C	2.14230456313097	6.09828632177542	3.93325238029980
H	1.54745172973776	6.75929682244805	3.31679080885812
C	1.74181547430463	5.79103509267617	5.23221932880584
H	0.82104573687031	6.21316039980895	5.61932230967780
C	2.51203495868353	4.92667490412069	6.01122156000152
H	2.19210788535870	4.67488341432220	7.01812644788232
C	3.68719596321581	4.37542640328336	5.49232948439870
H	4.28784082395314	3.70179418186346	6.09690379269278
C	4.10368087078224	4.69595388202851	4.20005735777742
H	5.01883223712330	4.28498709605904	3.78594689254971
C	3.91864136140546	8.39175711539920	2.55220884363843
C	3.23313989029124	9.50790506048330	2.04039768967439
H	2.82088353553260	9.45877838165092	1.03772794939484
C	3.10103536586489	10.66976187962367	2.79775647936101
H	2.57556775441453	11.52502684544853	2.38205614826597
C	3.63509447784090	10.73112258200657	4.08827696209408
H	3.53266926730292	11.63713292025762	4.67940612852822
C	4.29698962806369	9.61988425632196	4.61519928717512
H	4.71217070366550	9.65766926421867	5.61854320048456
C	4.44266230071288	8.46108521657016	3.85374022208096
H	4.97198105212340	7.60741743277175	4.26407735721092
C	5.03055321891814	8.09660138884544	-0.53798144300641
C	5.69569476338855	9.24891714413148	-0.08714540391708
H	5.85184500645663	9.39879194698688	0.97551510355718
C	6.17121557446741	10.19270478847482	-0.99562890696471
H	6.68570126459055	11.07728243779870	-0.62933942365212
C	6.00135436289078	9.99951598826646	-2.36840003618178
H	6.37314233472450	10.73696410090075	-3.07469661339531
C	5.35838209832679	8.84722819474349	-2.82655235153997
H	5.22761242260063	8.68420277502884	-3.89318557522782
C	4.87938214639663	7.90306348660158	-1.92097659864078
H	4.38415594652337	7.00181545177847	-2.26679650864539

Table S6. Geometry-optimized structures in Cartesian coordinates of PAI-InCz with B3LYP-D3/6-31G(d) by ORCA.

H	-2.76021092112201	4.57866208117730	6.01766134597651
C	-2.81522170455285	4.92576408162803	4.98967899693880
C	-1.77199735586517	5.68298651702787	4.44977475081656
H	-0.89998721466546	5.92993446152163	5.04654474514218
C	-1.83691973477872	6.11909084328334	3.12771024652688
H	-1.03462461339151	6.70394194319383	2.69562201168664
C	-2.95714933908849	5.80771654651402	2.35467880753350
C	-4.01107157661834	5.06523001157983	2.88919009089904
H	-4.86988799986758	4.83459886071187	2.26744094975901
C	-3.93265377122690	4.61871876911322	4.20876233548137
H	-4.74649688990709	4.03360455198285	4.62698775610336
N	-3.00039347992274	6.22439411896289	0.98985871515583
C	-2.90965722454442	5.38800914047190	-0.12452220821116
N	-2.95361854406530	6.07935660168088	-1.25036735496851
C	-3.06761118885052	7.39728284553432	-0.88054761370852
C	-3.11144374741107	7.52852798938074	0.50460375077249
C	-3.30865464877740	8.79049283288428	1.16088928011903
C	-3.38674434653419	9.94309385995090	0.30811356324825
C	-3.54201833474940	11.20239729687865	0.92731489294965
H	-3.58316477573031	12.09632669115277	0.31603433080460
C	-3.65593425218980	11.33996452787943	2.30083208254561
H	-3.77883409241327	12.32755969488394	2.73666123626071
C	-3.62988424195329	10.20206102875636	3.11999416684223
H	-3.73636382135585	10.29764693446729	4.19686645735021
C	-3.45626927171239	8.95140315597447	2.55703837698163
H	-3.42835641543186	8.08410446672570	3.20116482215631
C	-3.31731211949451	9.81434646230270	-1.15136974606308
C	-3.14818470822163	8.53419057644034	-1.74860048346482
C	-3.05828727470735	8.39696556148133	-3.14702559335047
H	-2.91527556709549	7.40133357603447	-3.55396110369426
C	-3.14346123336848	9.50752853396792	-3.96562830456869
H	-3.07071723320020	9.39953794737741	-5.04434602535034
C	-3.33113901709768	10.77877843319216	-3.39456216254762
H	-3.41002368583932	11.65484891763150	-4.03266191844269
C	-3.41635604717494	10.92462436811620	-2.02001449541645
H	-3.55975184842943	11.92070664005446	-1.61686786776462
C	-2.78824966896187	3.92437713005881	-0.08174684695181
C	-3.34642135406710	3.18435726109348	-1.14002111584866
H	-3.86258693972924	3.72035075137997	-1.92893581160740
C	-3.20777910338539	1.80091602144832	-1.20012117143211
H	-3.61298175879962	1.24109496198860	-2.03715180483110
C	-2.50846325334305	1.12267751005102	-0.19477553876291
C	-1.96893291686970	1.84768977356644	0.87541772066533
H	-1.42720462182387	1.31931164949028	1.65297966151249
C	-2.09863383170399	3.23075365457548	0.92734896107344
H	-1.65583593916366	3.77050336311238	1.75439286599588
N	-2.27006225595317	-0.27130293884483	-0.27837605615525
C	-0.99183061281196	-0.83223433823793	-0.25468512762451
C	0.22252933891404	-0.15890141576347	-0.25065627831865
H	0.28413486662102	0.92073563605787	-0.25454936631916
C	1.35150023213438	-0.96893860518771	-0.24168505826169
C	1.30084435552312	-2.39402889533006	-0.21024208317418
C	0.05954059772072	-3.03949619579275	-0.24785079999670
H	-0.00413260091321	-4.12439175153827	-0.24374510219213
C	-1.09970065800310	-2.25518100136935	-0.28137631806307
C	-2.52237145776063	-2.54732117926670	-0.34006241697528

C	-3.27855056799646	-3.72236238480871	-0.38504777229107
H	-2.78833543908890	-4.69247423831538	-0.38929050410246
C	-4.66696540311062	-3.64050921599814	-0.42245505492264
H	-5.23946323666186	-4.56211649874265	-0.46104917000257
C	-5.35031182938765	-2.40309262863677	-0.40963871870024
C	-4.60170388216005	-1.22191561127425	-0.36417223467604
H	-5.07952960971358	-0.25039531838950	-0.34471474915752
C	-3.21065413378811	-1.30690292790402	-0.33876035265571
C	-6.88541456971548	-2.39132310488219	-0.44813919557684
C	-7.36902749321204	-3.06975986975302	-1.74941137517482
H	-8.46526799197681	-3.07763930857440	-1.79223341408224
H	-7.02239748295083	-4.10588988762722	-1.81935520540777
H	-6.99542064854635	-2.53244670105825	-2.62839354856699
C	-7.43603961388315	-3.16605391426281	0.77002833905661
H	-8.53293143728151	-3.17357732789219	0.75378096698362
H	-7.10981415073072	-2.69948743832042	1.70649706983689
H	-7.09338916950379	-4.20561451922550	0.77747287694322
C	-7.46234019996205	-0.96588620787156	-0.40869280665538
H	-8.55687032393277	-1.01016543650467	-0.43583274653068
H	-7.17318869660800	-0.43702934544349	0.50659137947862
H	-7.13303956413479	-0.37046665294749	-1.26777276582840
C	2.68241755140541	-2.84045798600373	-0.11126391650242
C	3.50311641758833	-1.67826466948523	-0.08855322702058
C	4.88728381165731	-1.74505594692050	0.01023659635404
H	5.47160186399444	-0.83032807891284	0.01508883211722
C	5.50460035514137	-3.00254912692229	0.10064034038663
C	4.69563328171060	-4.15598862167219	0.07736769777070
H	5.15490481049298	-5.13472054981378	0.14493441917462
C	3.30525472519289	-4.08567342275688	-0.02975827871691
H	2.71570729057088	-4.99878570274425	-0.04553138211575
C	7.03472740195516	-3.07089453383790	0.22268412397613
C	7.55323319737572	-4.51538687035237	0.32598817510035
H	8.64548997831006	-4.50871897185614	0.41472337699253
H	7.15037643679376	-5.02780739098730	1.20680423472103
H	7.29583406629799	-5.10384732307479	-0.56180706501863
C	7.47979388609014	-2.30963865162718	1.49143748927908
H	8.57099564898815	-2.34833497497656	1.59825358332302
H	7.03114495809919	-2.75346514776978	2.38748016319156
H	7.18388469470097	-1.25612407113518	1.45482526648922
C	7.67904803914903	-2.41578041391336	-1.01927521429444
H	8.77311393723070	-2.44950391958644	-0.94543879636755
H	7.38212686435833	-1.36714450224844	-1.12474361625947
H	7.38074887765816	-2.94118043989634	-1.93345941326161
N	2.68482014717581	-0.55264576902634	-0.20125424094543
C	2.99493411444634	0.82746496522059	-0.10312127390782
C	2.59266966363356	1.66709292105654	-1.14984500756382
H	2.25160802136772	1.22308423982591	-2.07954959090368
C	2.51748464212848	3.03692104651076	-0.95452238634885
H	2.12496620376113	3.68887419417594	-1.72612223775099
C	2.86923731234724	3.60558665579653	0.28507063112993
C	3.43002078966488	2.76987039065977	1.26823957595425
H	3.77493444286454	3.17787546491442	2.20898355093348
C	3.47725120272712	1.38833420906003	1.08201194494880
H	3.81610936475887	0.73904095106267	1.88357536043550
C	2.49684331202506	5.01310389959753	0.47226379943134
N	2.17363489143771	5.80707693430849	-0.53567486284169
C	1.65493062753029	6.94628502944918	0.02269739987380
C	1.67543064874594	6.87537123024995	1.41230938610855
N	2.23520756836007	5.62634713922425	1.69984760298172

C	2.24040464472376	4.98806009566567	2.97827888707170
C	3.30315202306512	5.19432280549253	3.86031865147666
H	4.12003361442623	5.84465922032404	3.56335439253109
C	3.29025826083489	4.56854176088703	5.10715334704944
H	4.11292779229757	4.72681252700339	5.79826657230894
C	2.22237108017782	3.73986380655775	5.46458424369919
H	2.21594343305170	3.25348391365104	6.43571244742300
C	1.16646737553692	3.53450403173509	4.57366789745081
H	0.33352233600358	2.89418582898476	4.84820394459205
C	1.17448171258797	4.15837071639127	3.32651386418732
H	0.36960470243861	4.00752954987103	2.61613727588822
C	1.12725282168456	7.90152693478470	2.25369256471002
C	0.49125554301454	8.99908883486562	1.57802176656558
C	-0.15848961897630	9.96612068115395	2.37362831638385
H	-0.70528457259695	10.77070966580556	1.89827992381989
C	-0.16005462051479	9.90082638109718	3.75603668494484
H	-0.68800369061107	10.65803297007021	4.32758341222747
C	0.50609667224362	8.85394670291106	4.40881052161832
H	0.52230951224090	8.80520609819083	5.49425741458257
C	1.13612137534047	7.86937913146484	3.66826922524326
H	1.63354665492584	7.05881187504582	4.18263242183761
C	0.50186465222495	9.09944306256036	0.11444935976307
C	1.08576627654913	8.06511016173483	-0.66969913667848
C	1.07376921520303	8.13068282289512	-2.07567184163538
H	1.51189289808442	7.30771201387496	-2.63076567443493
C	0.51075771555220	9.21824556532084	-2.71715074705495
H	0.49032221435926	9.26495727336959	-3.80203022987308
C	-0.03932638802620	10.26446075439785	-1.95904674482895
H	-0.48929589763958	11.11551142098004	-2.45856002740288
C	-0.04744059468354	10.20228611879869	-0.57627354209941
H	-0.49368692317796	11.02116136554379	-0.02555639742040

Table S7. Geometry-optimized structures in Cartesian coordinates of CN-PAI-InCz with B3LYP-D3/6-31G(d) by ORCA.

H	-0.15270923378485	10.04849648242449	-1.00928291558336
C	-1.05999049688801	9.95706017686956	-0.41917756173655
C	-1.68290207043392	8.73002528410191	-0.28167884247570
H	-1.28387155404599	7.84317349611059	-0.76214427350552
C	-2.84703368944276	8.60264009063745	0.50207794064230
C	-3.41861425865760	9.73602403159678	1.14759736852882
C	-2.75538704493861	10.97329127054243	0.98438779297163
H	-3.13814363734060	11.86284926089413	1.47138232452483
C	-1.60194157721997	11.08385635929515	0.22445877410529
H	-1.11538763032582	12.05035597340460	0.12598493978055
C	-4.64245967312595	9.58959436620012	1.94565839733241
C	-5.22845539409330	8.29964820222177	2.17772622042731
C	-6.43095351005537	8.20217092078710	2.91273863513665
H	-6.89456326370507	7.23505782237369	3.05463917979682
C	-7.03987799147780	9.32777653719619	3.43717950594171
H	-7.96628985991071	9.23006284726688	3.99586495824829
C	-6.46496699900512	10.59101537852568	3.23427725756075
H	-6.94020388617059	11.47949821105091	3.63988494228329
C	-5.29792688193110	10.71022330357343	2.49900396602590
H	-4.89239230546624	11.70160976621936	2.33424788733658
C	-4.53855969319922	7.18039115330473	1.60290801018767
C	-3.45520915386726	7.32808455875460	0.74487817919065
N	-3.01302859419674	6.10505359210470	0.30360521654229
C	-3.76322165053489	5.19635935675507	0.90544276511100
N	-4.73729456106666	5.80044196287389	1.69649000377861
C	-5.67461289306592	5.11241536800790	2.51952178350994
C	-5.54046221528049	5.16700147445670	3.91089499716674
H	-4.72489667693581	5.73668803545902	4.34017240212409
C	-6.41760585192967	4.44274998723479	4.70939677960386
H	-6.32048438882669	4.46439061617954	5.78953052437557
C	-7.42236408286754	3.65648237610089	4.11711337534628
C	-8.30785360143068	2.88741760560717	4.94044107856763
N	-9.02297297374592	2.25862221201397	5.60824534058174
C	-7.55052745772637	3.61222869644445	2.71912885066454
H	-8.32702759067598	3.00298657264025	2.26922379836549
C	-6.67899689305445	4.34775791212642	1.92256667905291
H	-6.75781269648758	4.32110232289503	0.84107510669824
C	-3.46188915591927	3.76312141645153	0.83294893067209
C	-3.68675852284951	2.87065885223527	1.89542154682770
H	-4.13135670057531	3.21590262361451	2.81809118755547
C	-3.27756977043447	1.54533725792096	1.80349433101651
H	-3.43178730004558	0.86593005832965	2.63527984893390
C	-2.63160654036983	1.08115657414796	0.65289162512393
C	-2.38569037898514	1.96596291639988	-0.40552167658006
H	-1.89374688524093	1.59987181616329	-1.30100518071476
C	-2.79540988823529	3.29025684411313	-0.31314458802946
H	-2.61149080473747	3.98051401634965	-1.12935343875117
N	-2.24997375282883	-0.27571753218283	0.56028797968886
C	-0.96382924794313	-0.75703323206809	0.29481762998437
C	0.22019650722118	-0.03187114658619	0.15770410991723
H	0.24320244632182	1.04614935505281	0.25529279889724
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C	1.34340791688640	-2.21588387488515	-0.16264699247112
C	0.14676706213891	-2.91322103239293	0.00037825476162
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C	-4.50354467014162	-1.35592231417541	0.90122297055920
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H	-8.40526103489923	-1.34416426023915	1.54825962976407
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H	-7.19064194313561	-0.62551087459246	0.47969136080060
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C	3.51542343562401	-1.48381317106510	-0.43366803427451
C	4.88202000567438	-1.54894190957786	-0.68641055317232
H	5.46908725052374	-0.64079316763252	-0.75248201719159
C	5.48817545625735	-2.80190403211322	-0.86707932664398
C	4.68751729919864	-3.95852440283803	-0.79998931554357
H	5.13884139573657	-4.93394674204242	-0.93469064324584
C	3.31328475301598	-3.89023476198364	-0.57143649838957
H	2.72015505309373	-4.80050924572528	-0.54197534940552
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H	7.47362370294082	-1.14936665166779	0.16685335735850
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H	8.39508980672864	-2.12748461553967	-2.64757860776532
H	7.02074096944211	-1.04400233215330	-2.37532926075254
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C	3.13940990915909	0.98024800442380	-0.18572884667301
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H	1.60666141540082	1.71494290945772	-1.50848493372937
C	2.87941328552165	3.30217762170711	-0.81041670972456
H	2.35536853036650	4.06274354145894	-1.37751771829007
C	4.01158046934818	3.65380428243751	-0.05942279272576
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N	5.69109788450536	5.48015992681006	-0.19010146783431
C	5.63713995688015	6.85042919029717	-0.02225487730935

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C	2.38857291357200	5.84067411034338	2.41524533656056
H	3.34415865839664	5.89160235319430	2.92654350280835
C	1.20422403834157	5.70531286470834	3.13008084981559
H	1.21786259722476	5.64675411526415	4.21330192340736
C	-0.01877887765326	5.65114454640635	2.43994283534854
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H	-1.00164117086711	5.69784432722216	0.52197422184309
C	1.14254308924045	5.86884244775973	0.33522972575221
H	1.13385701491870	5.96200603600925	-0.74552683918105
C	3.99142960296576	8.63702353476701	0.50829902311378
C	5.05680316507840	9.59151877982019	0.40157298786403
C	4.73101279368466	10.95114444480800	0.60107960052353
H	5.50771394358575	11.70348536049589	0.52900511538589
C	3.43959786595420	11.36481553146141	0.88041462039723
H	3.23219141013091	12.42135143268710	1.02531913535427
C	2.40225149846315	10.42320154307552	0.96820338465143
H	1.38378200285901	10.73853801845660	1.17613155682510
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H	1.86739692530759	8.36488284405730	0.84517356284800
C	6.42407888949871	9.16462311668062	0.07931631844915
C	6.71423311927984	7.78715136571661	-0.14676850645167
C	8.01960317565895	7.36782775579269	-0.46994406207639
H	8.19033038985987	6.30884745257147	-0.63521838589255
C	9.04529140654736	8.28925112801748	-0.56901827530721
H	10.05155821592531	7.96347880779927	-0.81748272997998
C	8.77941196544559	9.65175479611340	-0.34599035885358
H	9.58165266900766	10.38060955230462	-0.42169128383861
C	7.49937335456940	10.07568256523332	-0.03066478721621
H	7.33402553875477	11.13437575451483	0.13362633943811

Computational details

ORCA computation package is use for all the calculations in this research. The molecular structures were geometrically optimized using dispersion-corrected density functional theory (DFT-D3) calculations with B3LYP/6-31G(d) functional and basis set. Molecular orbitals and their energy levels were calculated for the optimized structures by single-point energy calculations with B3LYP-D3/6-31G(d). Time-dependent density functional theory (TDDFT) calculations were studied under the same conditions and Tamm-Dancoff approximation (TDA).