Supporting Information

Rational Understanding of Substituent Effects on Multi Carbazole Thermally Activated Delayed Fluorescent Emitters

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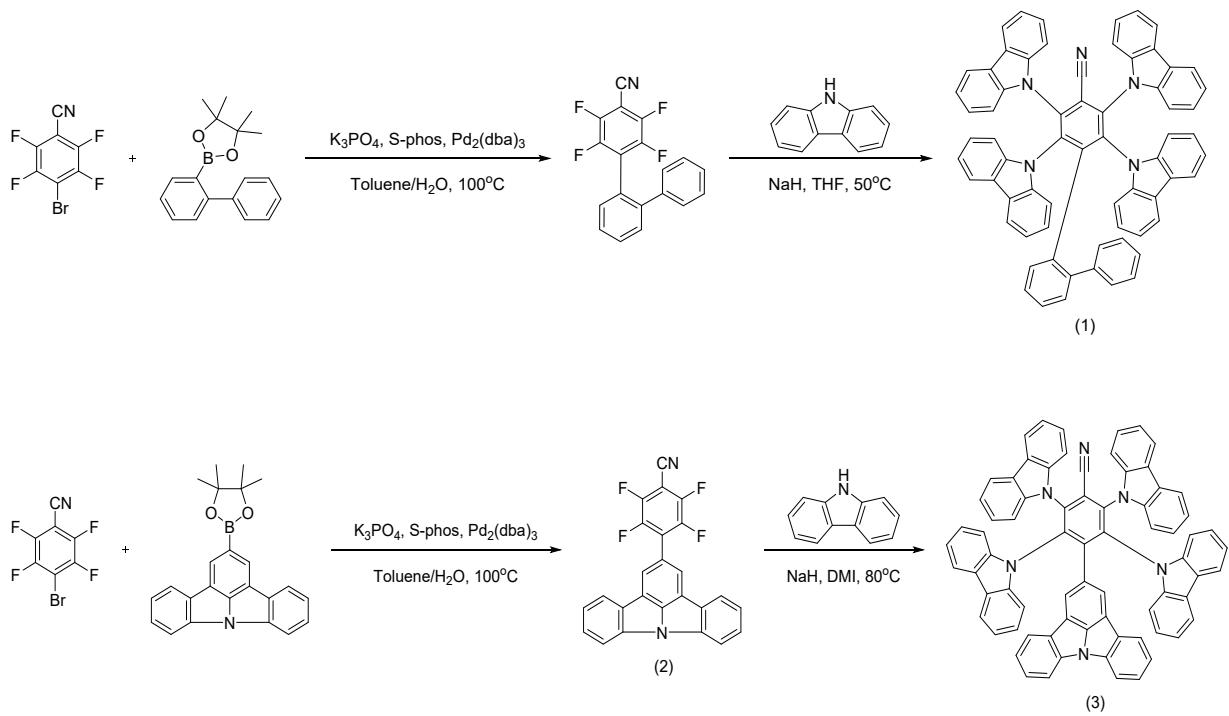
Scheme S1. Synthesis of 4CzBN-BP and 4CzBN-IDCz.

Experimental Section

Materials. All starting materials were commercially available from Aldrich, Alfa Aesar and TCI and were used without further purification. All solvents were purified prior to use and were purified by passage under a nitrogen atmosphere.

Characterization. ^{1}H NMR spectra were recorded using a Bruker 300 MHz spectrometer and and ^{13}C NMR spectra were recorded using a Bruker DRX 500 MHz spectrometer. High resolution mass analysis was measured using a Joel JMS-700. Thermal analysis was performed using a TA 2050 TGA thermogravimetric analyzer under a nitrogen atmosphere at a heating rate of 10 °C/min. Differential scanning calorimeter (DSC) was conducted under nitrogen atmosphere using a TA instrument 2100 DSC. The samples were heated at 10 °C/min from 10 °C to 400 °C. Cyclic voltammetry (CV) was performed at a room temperature in a 0.1 M solution of tetrabutylammonium perchlorate (Bu_4NClO_4) in chloroform under nitrogen gas at a scan rate of 50 mV/s. A Pt wire was used as the counter electrode and an Ag/AgCl electrode as the reference electrode.

Synthesis of [1,1':2',1''-terphenyl]-4-carbonitrile (BN-p-BP).

The reaction followed by literature method.[1] The crude material was isolated by column chromatography using DCM/n-hexane (1:6) as eluent to give a white solid (BN-p-BP). (3 g, 70% yield). ^{1}H NMR (300 MHz, CD_2Cl_2): δ = 7.56-7.46 (m, 6H), 7.30-7.26 (m, 5H), 7.16-7.13 (m, 2H).

Synthesis of 2,3,5,6-tetra(9H-carbazol-9-yl)-[1,1':2',1''-terphenyl]-4-carbonitrile (1) (4CzBN-BP)

9H-carbazole (1.87 g, 11.16 mmol) and sodium hydride (60% dipersion in mineral oil, 0.27 g, 11.16 mmol) were dissolved in tetrahydrofuran (15 mL). The solution was stirred for 1 h at 50 °C under nitrogen atmosphere. (2,3,5,6-Tetrafluoro-[1,1':2',1"-terphenyl]-4-carbonitrile (0.61 g, 1.86 mmol) was added to the solution, then yellow solid was obtained. The yellow solid was filtered and washed with water three times and washed with methanol for remained 9H-Carbazole. The crude product was purified by column chromatography using dichloromethane/hexane (1/1). (yield: 0.76 g, 44.7%) ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) = 7.83 (d, 2H, *J=7.4 Hz*), 7.72 (dd, 4H, *J=8.1Hz, J=9.4Hz*), 7.60 (d, 2H, *J=8.2Hz*), 7.52 (d, 2H, *J=7.8Hz*), 7.42 (t, 2H, *J=8.3Hz*), 7.379-7.306 (m, 5H), 7.296-7.204 (m, 4H), 7.193-7.102 (m, 4H), 7.066-6.928 (m, 8H), 6.79 (m, 3H), 6.45 (dq, 3H, *J=1.3Hz, J=8.3Hz*), 6.33 (d, 1H, *J=8.3Hz*) ^{13}C NMR (500mHz, $CDCl_3$) δ 150.14, 141.15, 139.98, 139.83, 139.47, 138.95, 138.89, 138.79, 131.14, 130.5, 129.98, 129.09, 128.96, 128.83, 127.79, 125.99, 125.63, 125.17, 125.11, 124.98, 123.88, 123.83, 123.55, 122.76, 121.06, 120.76, 120.63, 120.23, 119.88, 119.78, 119.67, 118.82, 117.79, 112.76, 110.56, 110.31, 110.16 HRMS (EI, m/z): calcd for $C_{67}H_{41}N_5$ 915.3362, found 916.3445.

Synthesis of 2,3,5,6-tetrafluoro-4-(indolo[3,2,1-jk]carbazol-2-yl)benzonitrile (2) (4FBN-ICz)

4-Bromo-2,3,5,6-tetrafluorobenzonitrile (3.00 g, 11.8 mmol) and 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)indolo[3,2,1-jk]carbazole (6.51 g, 17.6 mmol) were dissolved in toluene/H_2O (100 mL/25 mL). 2-Dicyclohexyl phosphino-2',6'-dimethoxybiphenyl (S-phos) (0.728 g, 1.76 mmol) and K_3PO_4 (7.522 g, 35.4 mmol) added to the solution, and then bubbling with nitrogen for 20 min. $Pd_2(dba)_3$ (0.54 g, 0.58 mmol) put into the reaction flask, the mixture was stirred for 12 h at 100 °C under nitrogen atmosphere. After cooling down to room temperature, dichloromethane and water were added to the reaction mixture. The phase was

separated and the aqueous layer was extracted with dichloromethane for three times. The combined organic phase was dried over anhydrous $MgSO_4$. The crude product purified by column chromatography using dichloromethane/hexane (2/1) (yield: 0.98 g, 20%) ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) = 8.25 (ddd, 1H, *J=0.8Hz, J=1.2Hz, J=7.8Hz*), 8.20 (t, 2H, *J=1.6Hz*), 8.05 (td, 2H, *J=0.8Hz, J=8.1Hz*), 7.70 (t, 2H, *J=7.8Hz*), 7.48 7.48 (dt, 2H, *J=1.0Hz, J=7.8Hz*) HRMS (EI, m/z): calcd for $C_{25}H_{10}F_4N_2$ 414.0780, found 414.0771.

Synthesis of 2,3,5,6-tetra(9H-carbazol-9-yl)-4-(indolo[3,2,1-jk]carbazol-2-yl)benzonitrile (3) (4CzBN-ICz)

9H-carbazole (1.93 g, 11.52 mmol) and sodium hydride (60% dispersion in mineral oil, 0.55 g, 23.04 mmol) were dissolved in 1,3-dimehtyl-2-imidazolidinone (20 mL). The solution was stirred for 4 h at 80 °C under nitrogen atmosphere. 2,3,5,6-tetrafluoro-4-(indolo[3,2,1-jk]carbazol-2-yl)benzonitrile (0.8 g, 1.92 mmol) was added to the solution, then the solid was precipitated. The obtained solid was filtered and washed with water three times and washed with methanol for remained 9H-carbazole. The crude product was purified by column chromatography using dichloromethane/hexane (2/3). (yield: 1.00 g, 51.55%) ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) = 7.88 (d, 4H, *J=7.4Hz*), 7.62 (d, 2H, *J=8.0Hz*), 7.48 (dd, 8H, *J=8.0Hz, J=10.1Hz*), 7.38 (t, 2H, *J=7.7Hz*), 7.332-7.186 (m, 20H), 7.14 (dd, 2H*, J=6.6Hz, J=7.6Hz*), 7.05 (t, 4H*, J=7.8Hz*), 6.89 (t, 4H, *J=7.5Hz*) ^{13}C NMR (500mHz, CD_2Cl_2) δ 150.139, 141.143, 139.978, 139.835, 139.471, 138.946, 138.897, 138.793, 131.138, 130.357, 129.980, 129.096, 128.963, 128.835, 127.799, 125.991, 125.632, 125.171, 125.114, 124.985, 123.886, 123.836, 123.556, 122.759, 121.062, 120.758, 120.631, 120.230, 119.880, 119.787, 119.668, 118.823, 117.797, 112.755, 110.562, 110.294, 110.162. HRMS (EI, m/z): calcd for $C_{73}H_{42}N_6$ 1002.3471, found 1003.3539.

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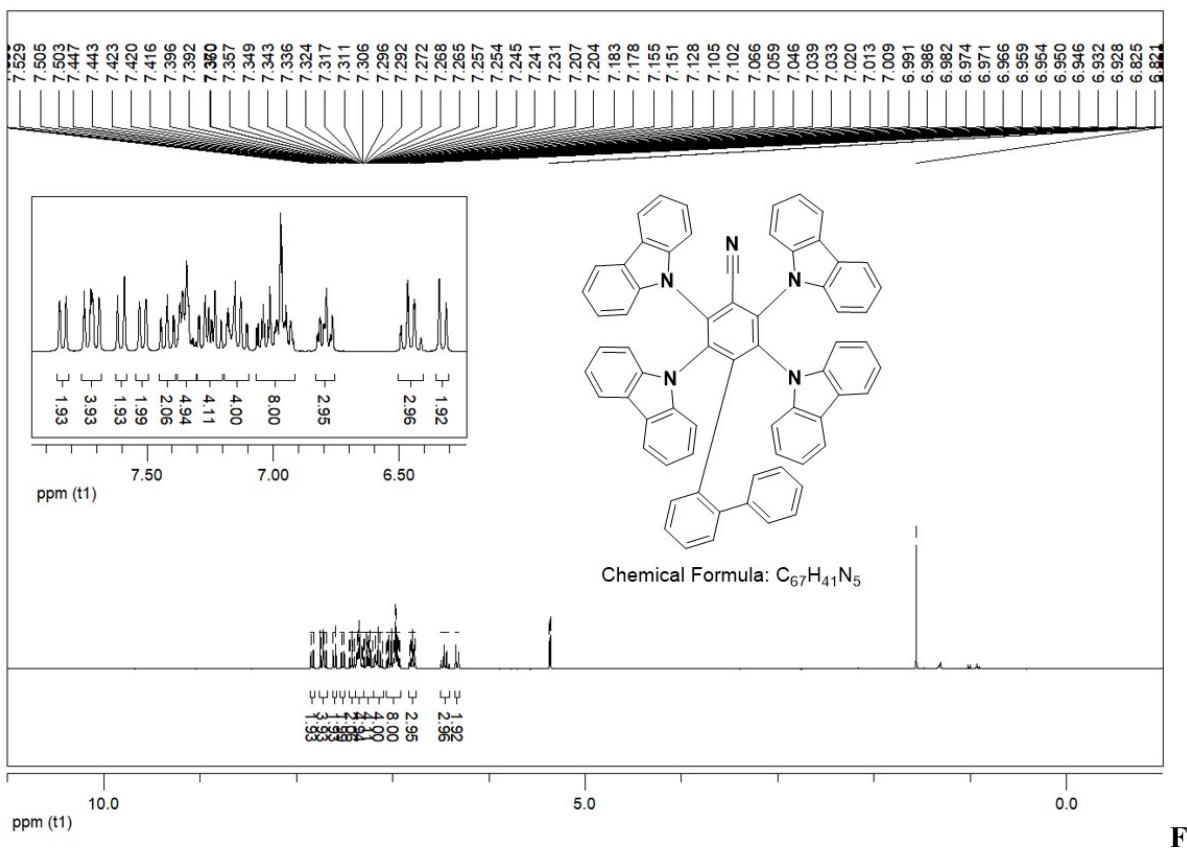
igure S1. ^{1}H-NMR spectra of 4CzBN-BP (1)
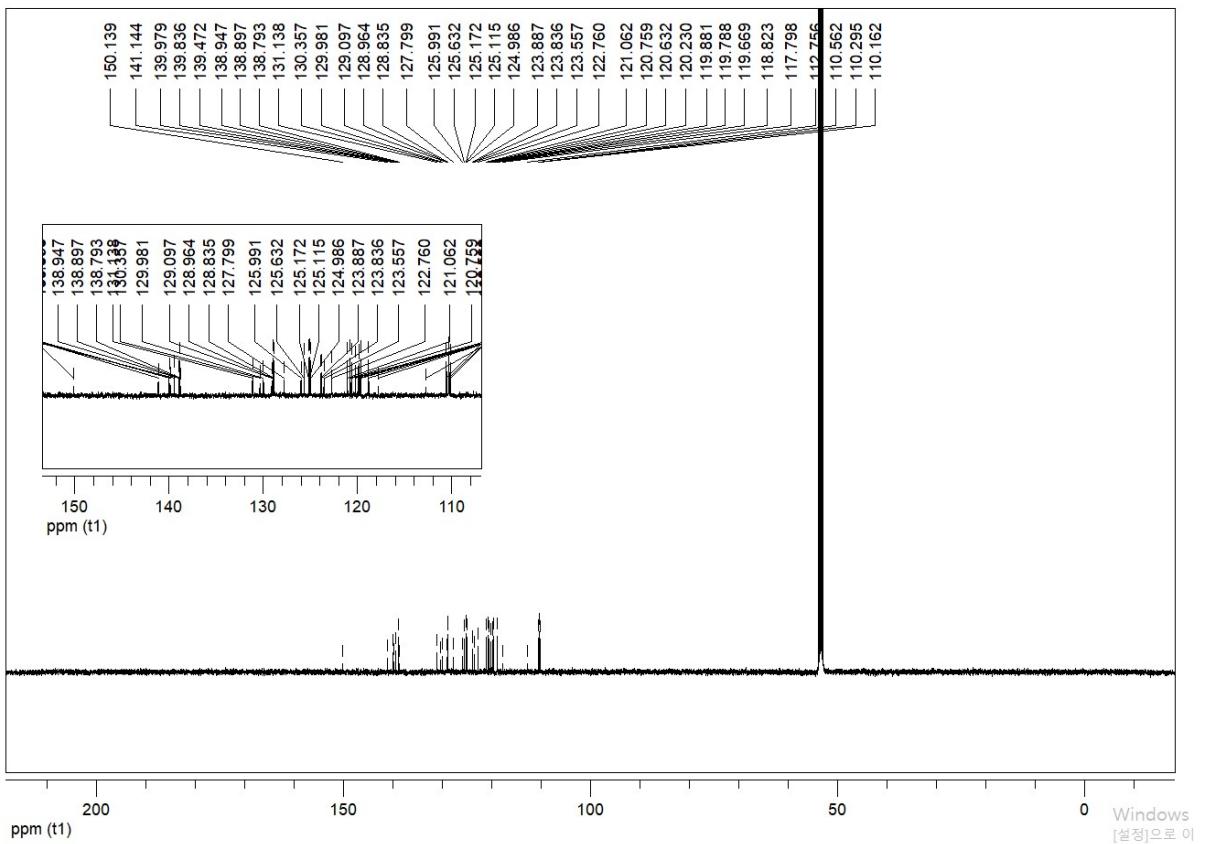
Figure S2. ^{13}C-NMR spectra of 4CzBN-BP (1)
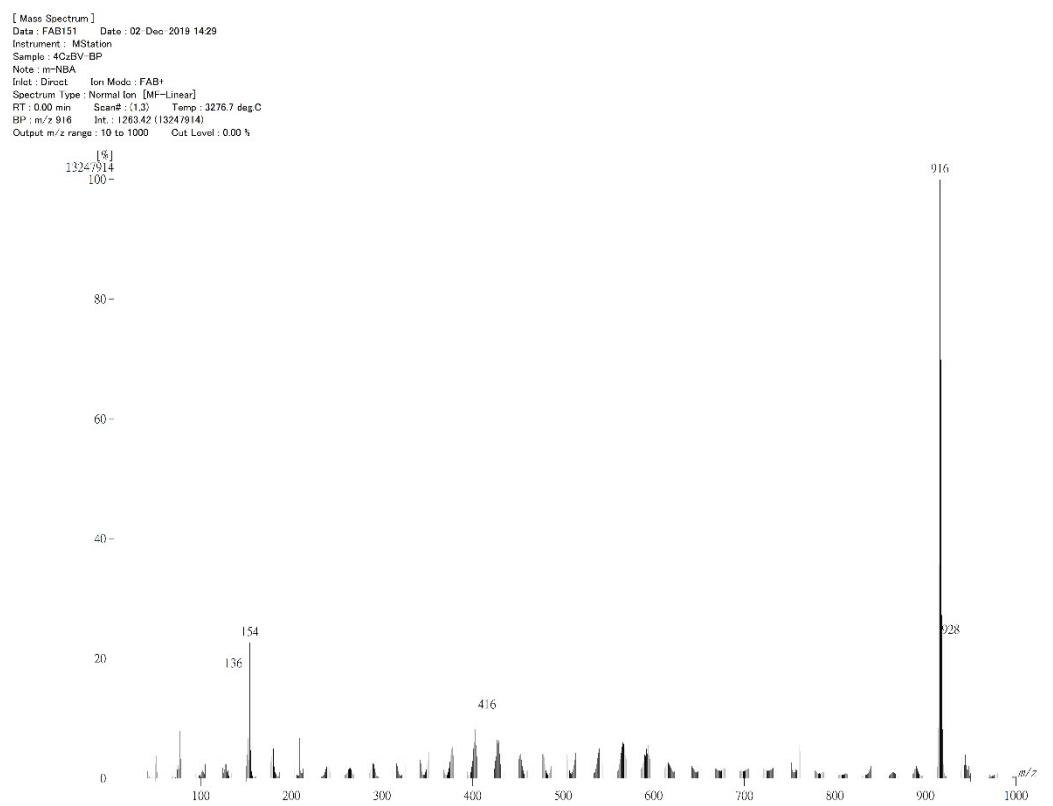
Figure S3. Mass spectrum of 4CzBN-BP (1)
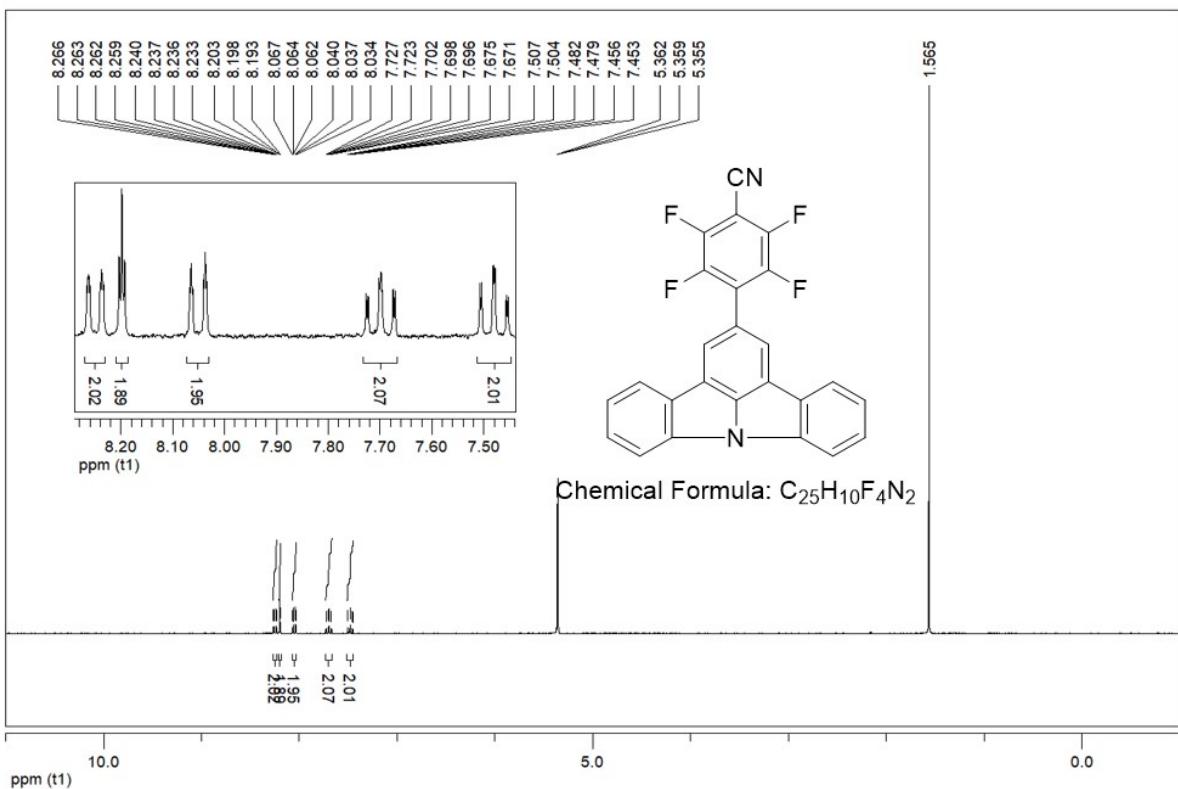
Figure S4. ^{1}H-NMR spectra of 4FBN-ICz
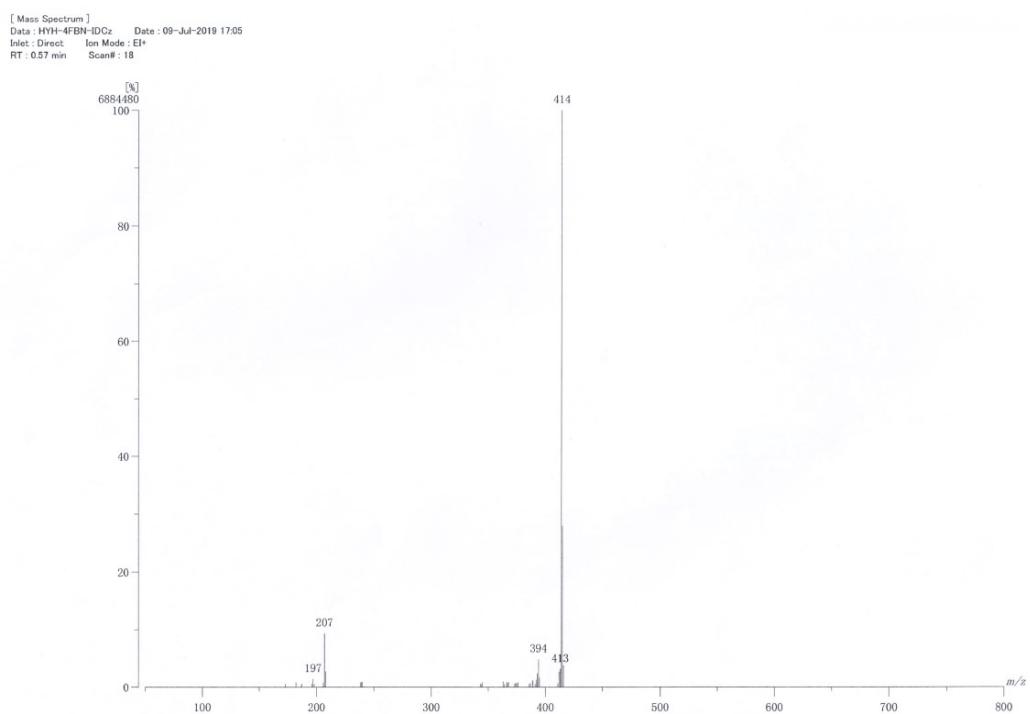
Figure S5. Mass spectrum of 4FBN-ICz

Figure S6. ^{1}H-NMR spectra of 4CzBN-ICz (2)
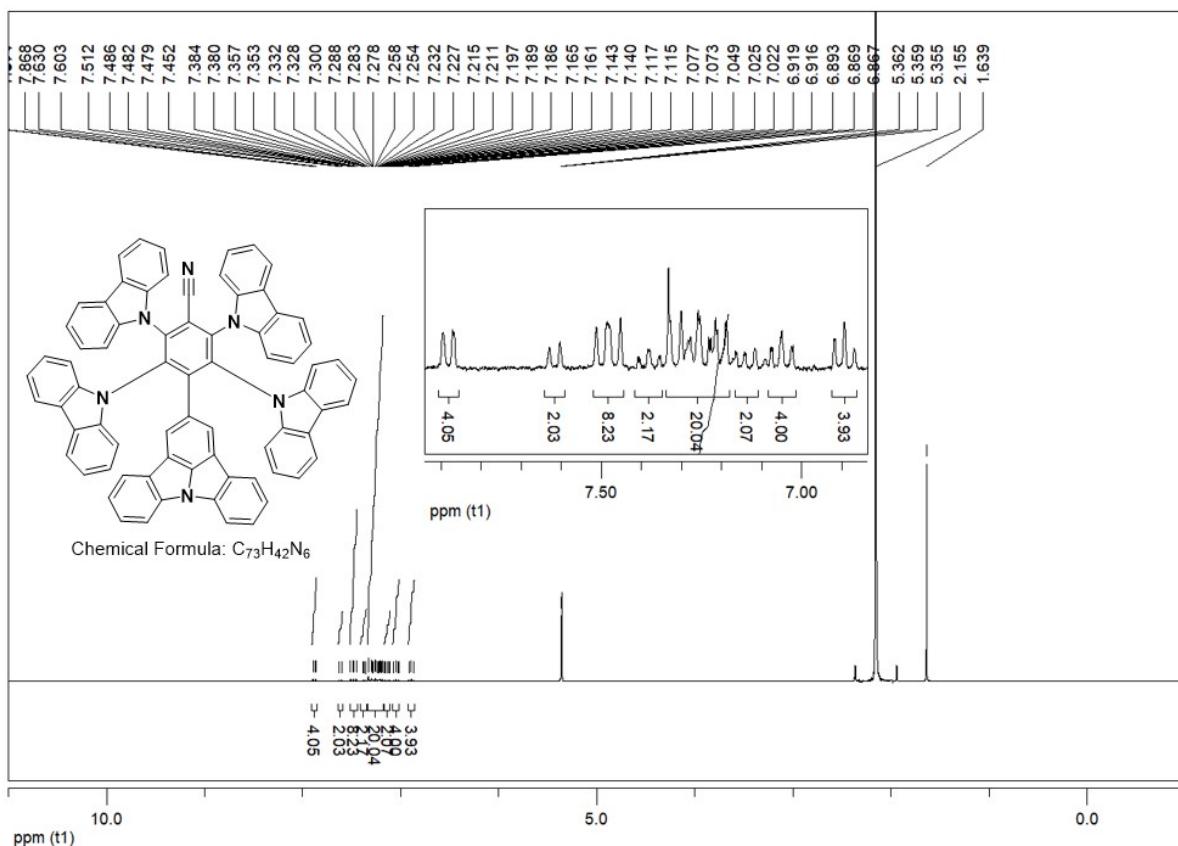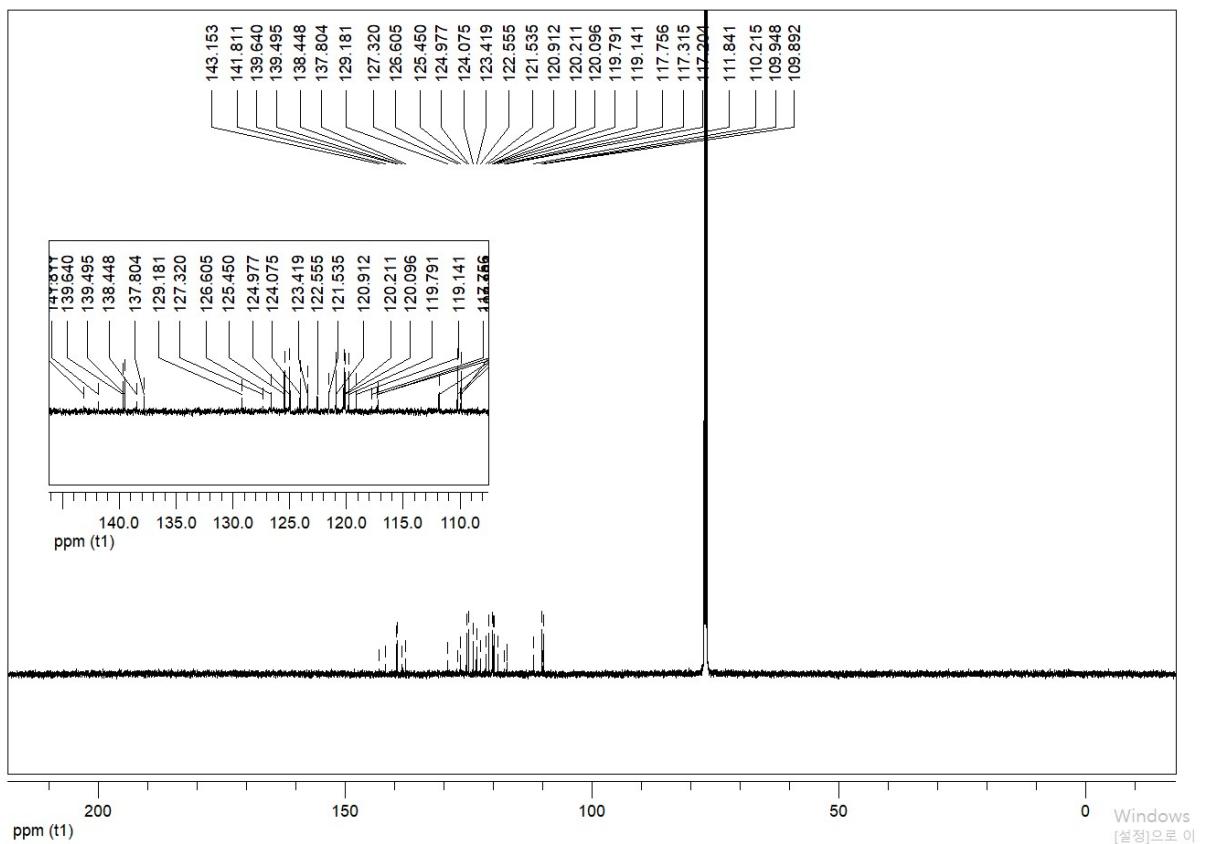
Figure S7. ^{13}C-NMR spectra of 4CzBN-ICz (2)
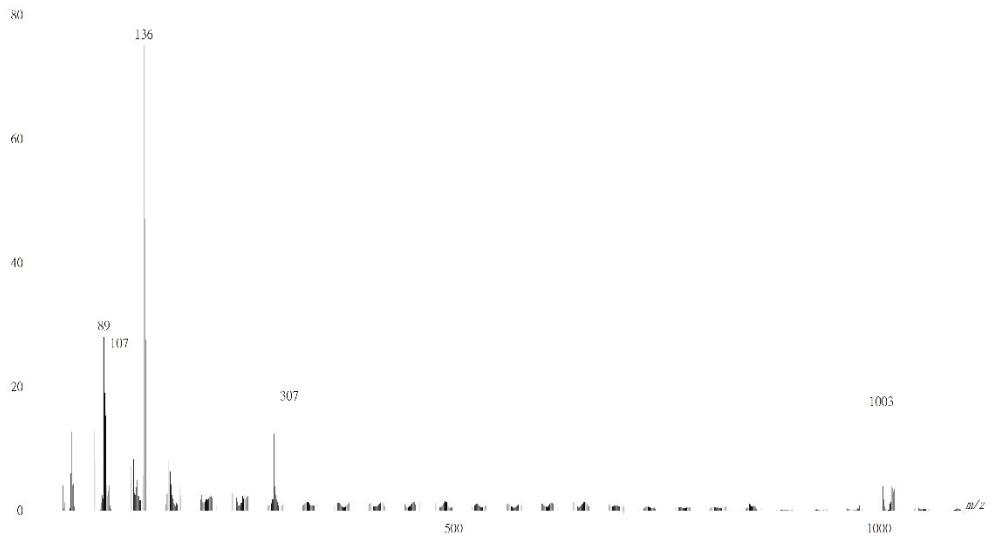
Figure S8. Mass spectrum of 4CzBN-ICz (2)
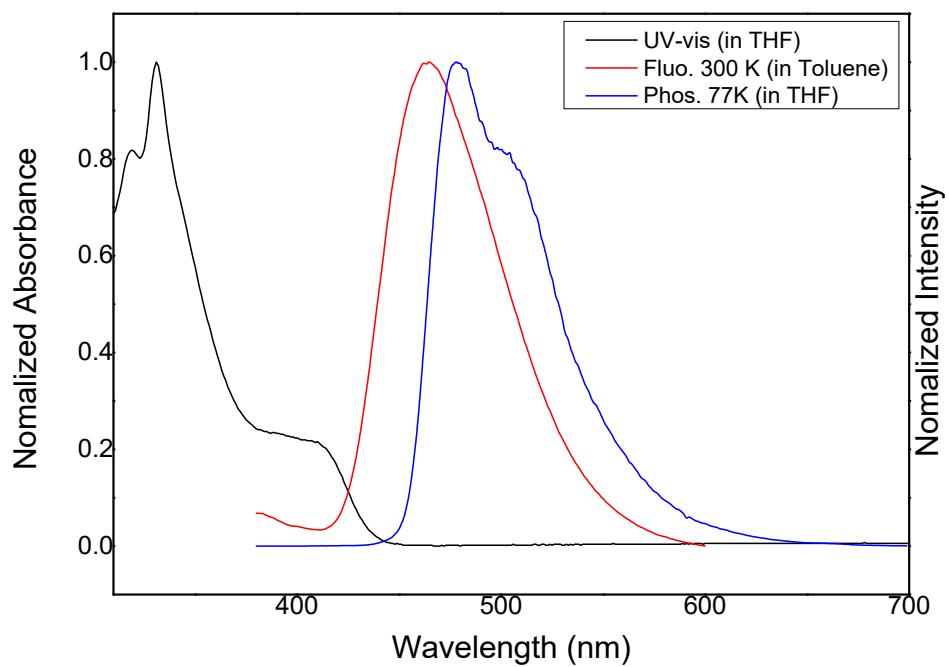
Figure S9. Absorption and photoluminescence spectra of 4CzBN-BP
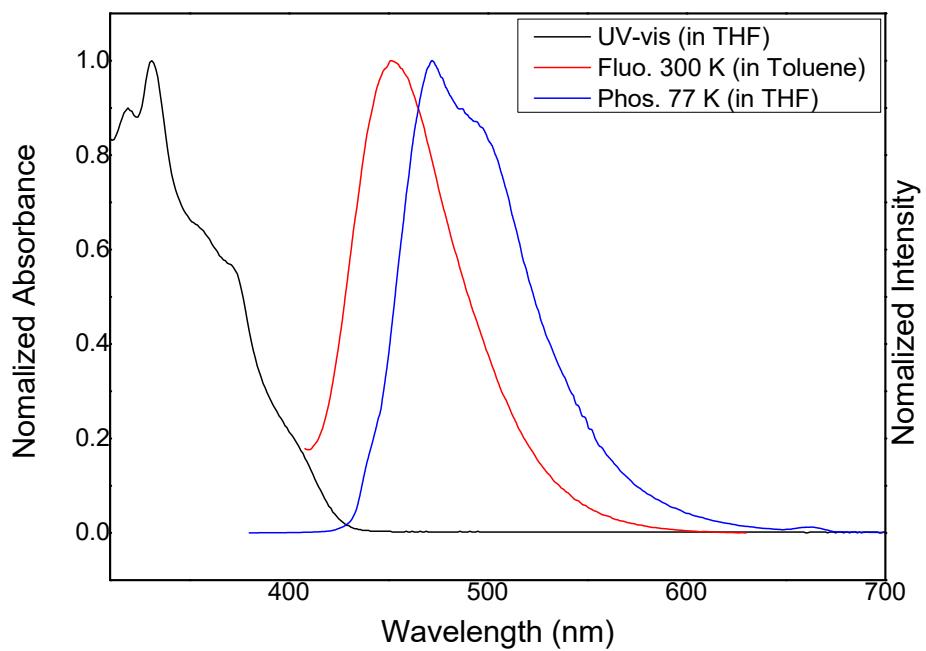
Figure S10. Absorption and photoluminescence spectra of 4CzBN-ICz
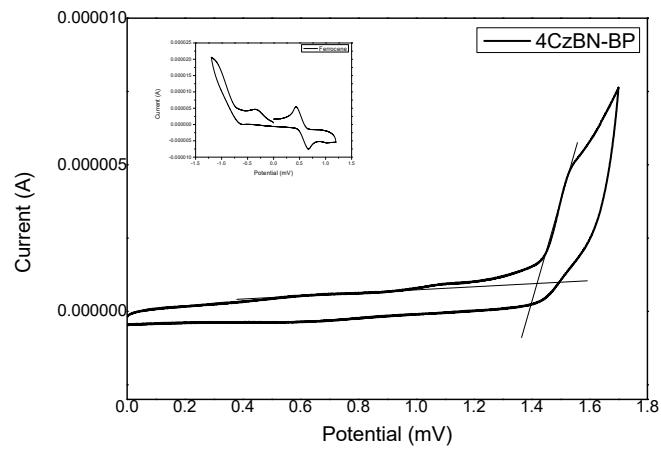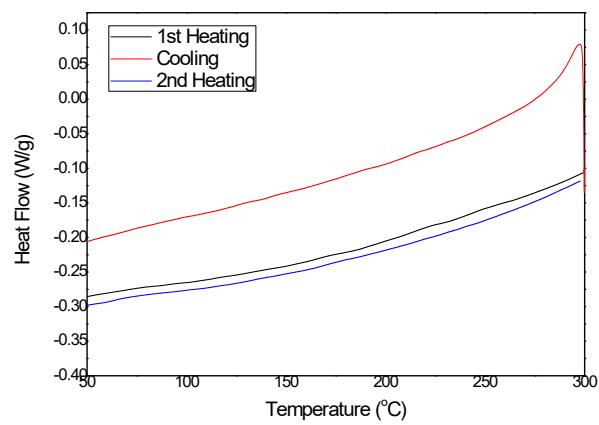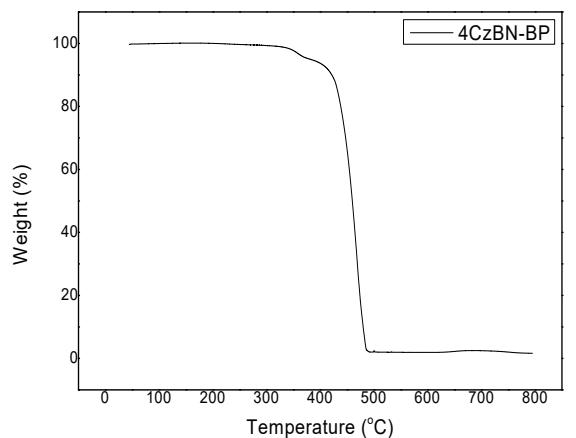
Figure S11. Thermogravimetric ananlysis (TGA), differential scanning calorimetry (DSC) and cyclic voltammetry (CV) results of 4CzBN-BP
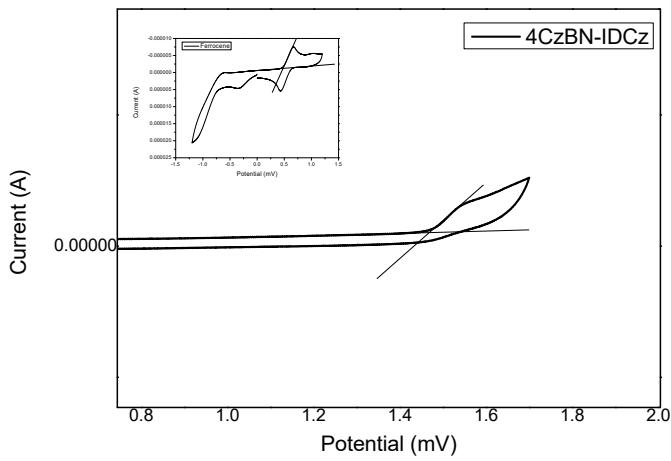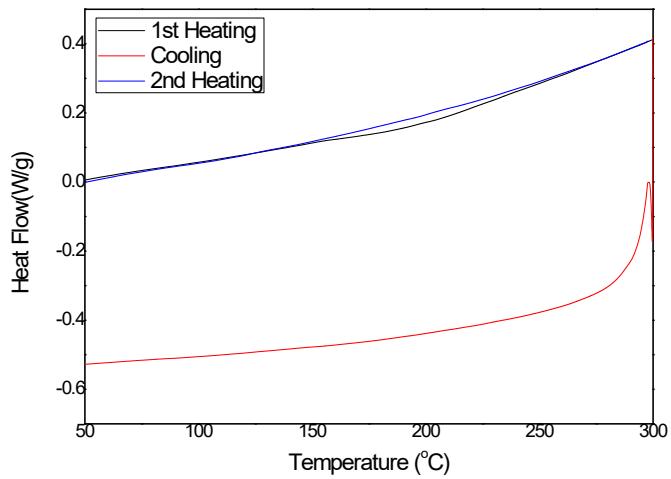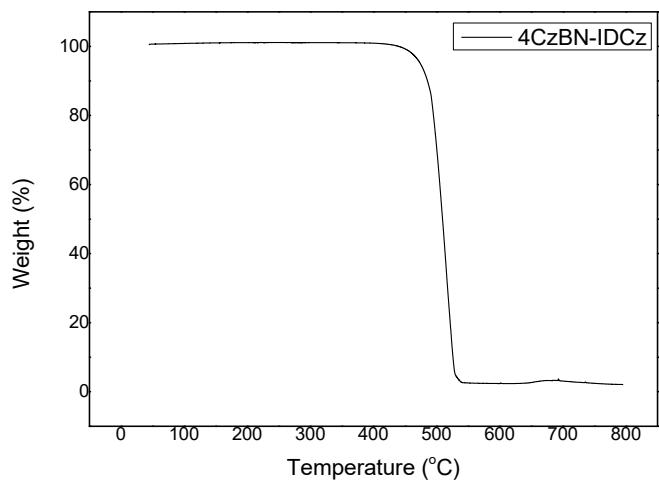
Figure S12. Thermogravimetric ananlysis (TGA), differential scanngin calorimetry (DSC) and cyclic voltammetry (CV) results of 4CzBN-ICz
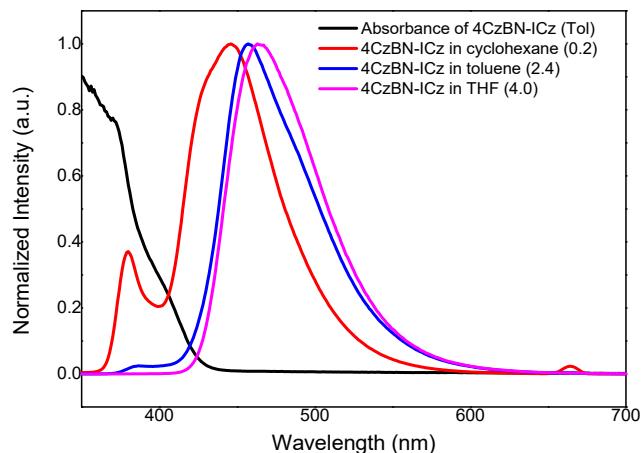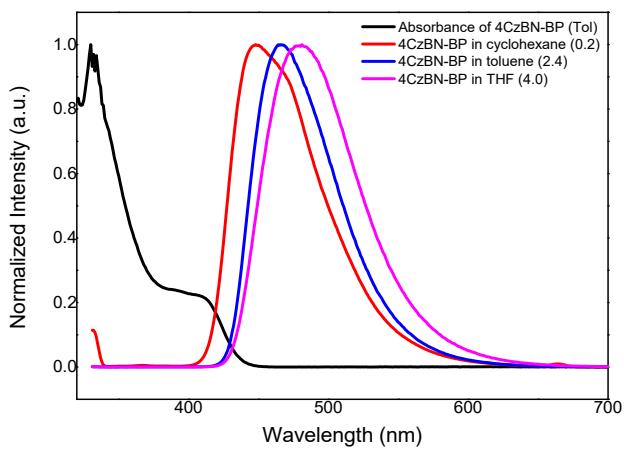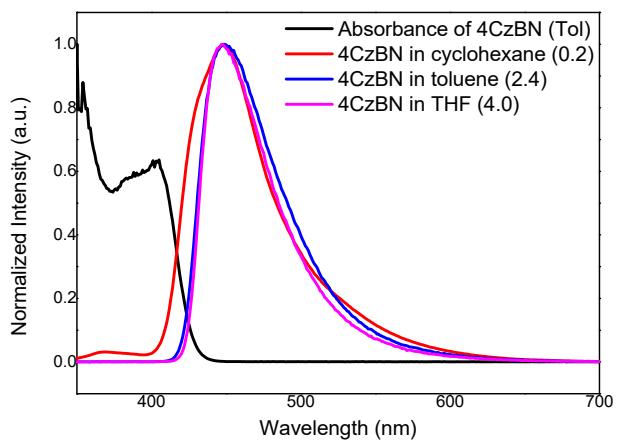
Figure S13. The solvatochromic characteristics of the 4CzBN, 4CzBN-BP, and 4CzBN-ICz in cyclohexane, toluene, and THF.
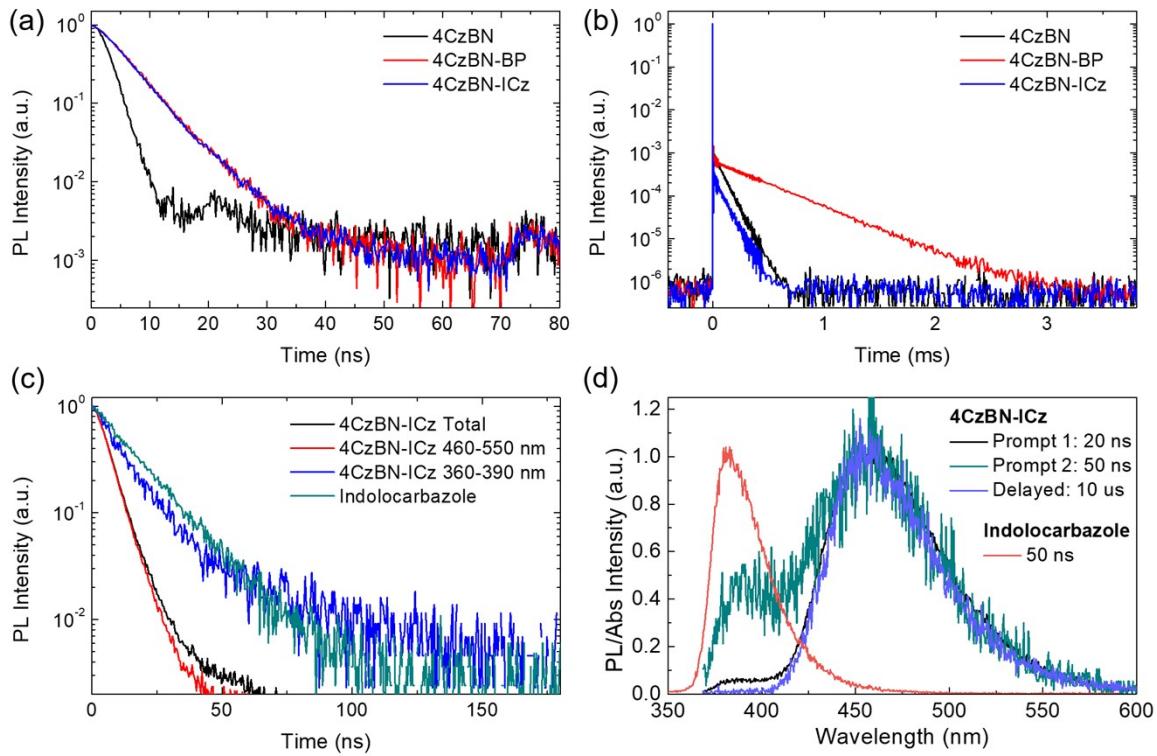
Figure S14. PL decay and time-resolved spectra of 4CzBN-Icz and indolocarbazole in toluene (10^{-5} M, N_2 purged). Excitation: 337 nm pulsed laser. (a) Transient PL decay of prompt fluorescence. (b) Transient PL decay of total emission. (c) Wavelength dependent PL decay of 4CzBN-ICz and indolocarbazole. (d) Time-resolved spectra of 4CzBN-ICz and indolocarbazole.
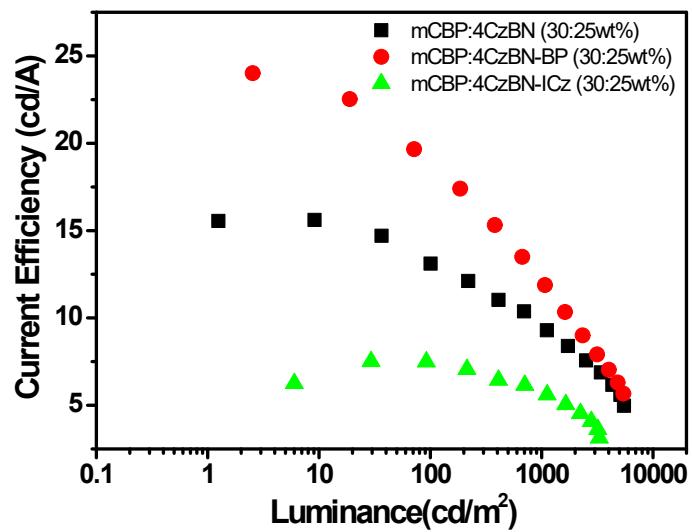
Figure S15. Current efficiency (CE) of the blue TADF OLEDs as the function of luminance.

Table S1. Geometry Coordinates of Relaxed Geometries of TADF Molecules

4CzBN S$_0$

C1	1.00E-04		1.3823	-1.00E-04
C2	-1.2261		0.7133	0.0152
C3	-1.2393		-0.6989	0.01
C4	0		-1.3843	0
C5	1.2393		-0.6989	-0.0101
C6	1.2262		0.7132	-0.0154
C7	0		-2.818	1.00E-04
N8	0		-3.9804	1.00E-04
N9	2.4451		-1.432	-0.0122
C10	2.9097		-2.2599	1.0274
C11	4.1581		-2.8068	0.648
C12	4.4566		-2.3081	-0.6794
C13	3.3845		-1.4658	-1.0587
N14	2.4106		1.485	-0.0707
C15	2.6971		2.4202	-1.0799
C16	3.8963		3.0968	-0.75
C17	4.3387		2.5746	0.5267
C18	3.3978		1.5934	0.9248
C19	-3.8962		3.0967	0.7498
C20	-2.6969		2.4203	1.0797
N21	-2.4105		1.4851	0.0705
C22	-3.3978		1.5932	-0.9249
C23	-4.3387		2.5744	-0.5268
C24	-4.1582		-2.8067	-0.6478
C25	-4.4566		-2.3078	0.6796
C26	-3.3844		-1.4655	1.0588
N27	-2.445		-1.4319	0.0122
C28	-2.9097		-2.2599	-1.0273
C29	5.5147		-2.5172	-1.5706
C30	5.485		-1.895	-2.8155
C31	4.4054		-1.0735	-3.1787
C32	3.3389		-0.8507	-2.3093
C33	2.3334		-2.5344	2.2685
C34	3.0283		-3.3791	3.1327
C35	4.2666		-3.9342	2.7721
C36	4.836		-3.6517	1.5335

C37	5.4189		2.8746	1.364
C38	5.538		2.2091	2.5805
C39	4.5831		1.255	2.9681
C40	3.4995		0.9372	2.1513
C41	2.0008		2.6944	-2.2594
C42	2.5238		3.6673	-3.1105
C43	3.7118		4.348	-2.7989
C44	4.4019		4.0662	-1.6228
C45	-3.4996		0.937	-2.1513
C46	-4.5834		1.2546	-2.9681
C47	-5.5383		2.2086	-2.5804
C48	-5.4192		2.8742	-1.364
C49	-4.4019		4.0662	1.6227
C50	-3.7117		4.3481	2.7986
C51	-2.5235		3.6675	3.1101
C52	-2.0005		2.6946	2.259
C53	-5.5147		-2.5168	1.5708
C54	-5.4849		-1.8944	2.8157
C55	-4.4053		-1.073	3.1787
C56	-3.3388		-0.8504	2.3093
C57	-2.3334		-2.5347	-2.2683
C58	-3.0285		-3.3794	-3.1325
C59	-4.2668		-3.9343	-2.7717
C60	-4.8361		-3.6516	-1.5332
H61	1.00E-04		2.4668	-2.00E-04
H62	6.3448		-3.1622	-1.2953
H63	6.3008		-2.0493	-3.5158
H64	4.3967		-0.6	-4.1564
H65	2.509		-0.2174	-2.6031
H66	1.3714		-2.1202	2.5537
H67	2.5961		-3.615	4.1011
H68	4.7822		-4.5915	3.4662
H69	5.7958		-4.0797	1.2569
H70	6.1496		3.6235	1.0702
H71	6.3725		2.4318	3.2392
H72	4.6872		0.7491	3.9239
H73	2.7716		0.1986	2.4656
H74	1.0805		2.176	-2.51

H75	1.9976		3.9008	-4.0319
H76	4.0939		5.1008	-3.4822
H77	5.3224		4.5923	-1.3843
H78	-2.7716		0.1984	-2.4657
H79	-4.6875		0.7487	-3.9238
H80	-6.3728		2.4312	-3.239
H81	-6.1498		3.6231	-1.0701
H82	-5.3225		4.5921	1.3843
H83	-4.0937		5.1009	3.4819
H84	-1.9973		3.9011	4.0314
H85	-1.0801		2.1764	2.5096
H86	-6.3448		-3.1618	1.2956
H87	-6.3008		-2.0486	3.516
H88	-4.3965		-0.5994	4.1563
H89	-2.5088		-0.2171	2.603
H90	-1.3714		-2.1205	-2.5536
H91	-2.5963		-3.6155	-4.1008
H92	-4.7824		-4.5917	-3.4658
H93	-5.7959		-4.0796	-1.2566

4CzBN-BP S$_0$

C1	0.1208	-1.0837	0.1278
C2	-1.1155	-0.3878	0.1359
C3	-1.154	0.9925	-0.1592
C4	0.0551	1.6805	-0.394
C5	1.3022	1.0306	-0.2671
C6	1.3328	-0.3549	9.00E-04
C7	0.0225	3.0772	-0.715
N8	-7.00E-04	4.2079	-0.9842
N9	2.4838	1.7981	-0.3718
C10	2.8931	2.7959	0.5344
C11	4.1261	3.3299	0.0987
C12	4.4685	2.6561	-1.1369
C13	3.4362	1.7279	-1.4027
N14	2.5893	-0.9801	0.2503
C15	3.3109	-1.8915	-0.541
C16	4.4751	-2.285	0.1616

C17	4.4521	-1.6086	1.4397
C18	3.2783	-0.8227	1.4653
C19	-3.8153	-2.0446	1.9601
C20	-2.5063	-1.5234	1.8567
N21	-2.2944	-1.0656	0.5419
C22	-3.4882	-1.2616	-0.1802
C23	-4.4386	-1.8789	0.665
C24	-4.0606	3.0351	-1.0291
C25	-4.1938	2.9529	0.4109
C26	-3.1346	2.1429	0.8805
N27	-2.3708	1.7127	-0.2191
C28	-2.9216	2.2781	-1.3824
C29	5.5292	2.7862	-2.0409
C30	5.5606	2.0128	-3.2012
C31	4.5016	1.1142	-3.4481
C32	3.4345	0.9628	-2.5679
C33	2.2769	3.2553	1.6993
C34	2.9195	4.2539	2.4243
C35	4.155	4.8032	2.0212
C36	4.7505	4.3311	0.8522
C37	5.2988	-1.6263	2.5544
C38	4.9801	-0.8815	3.6899
C39	3.7899	-0.1243	3.6925
C40	2.9304	-0.0842	2.5981
C41	3.0446	-2.4034	-1.8125
C42	3.9536	-3.3005	-2.3648
C43	5.1251	-3.7035	-1.6909
C44	5.3745	-3.1852	-0.4217
C45	-3.7934	-0.9725	-1.5099
C46	-5.0668	-1.29	-1.9699
C47	-6.0405	-1.8981	-1.1495
C48	-5.71	-2.1956	0.1714
C49	-4.2674	-2.5493	3.1847
C50	-3.4361	-2.5258	4.3047
C51	-2.1461	-1.9706	4.1782
C52	-1.6677	-1.4665	2.9715
C53	-5.0926	3.5119	1.3271
C54	-4.9367	3.2785	2.6932
C55	-3.8586	2.4791	3.1281

C56	-2.9496	1.9078	2.2425
C57	-2.5119	2.1593	-2.7113
C58	-3.2619	2.8155	-3.6825
C59	-4.4048	3.5796	-3.3647
C60	-4.7966	3.6804	-2.0299
C61	-2.0367	-3.8365	-2.5038
C62	-0.9697	-3.0681	-2.0006
C63	-0.512	-2.0039	-2.7978
C64	-1.0681	-1.7427	-4.0509
C65	-2.1094	-2.532	-4.5395
C66	-2.5964	-3.5761	-3.7525
C67	0.7654	-3.0986	1.4371
C68	0.8755	-4.4684	1.6523
C69	0.3914	-5.3486	0.6885
C70	-0.1951	-4.8455	-0.4676
C71	-0.3339	-3.4647	-0.7063
C72	0.1682	-2.5748	0.2803
H73	6.3268	3.4986	-1.8435
H74	4.5169	0.5192	-4.3583
H75	2.6299	0.2713	-2.7917
H76	1.3192	2.8657	2.03
H77	2.4478	4.6275	3.3302
H78	5.7012	4.7448	0.5239
H79	6.2052	-2.2273	2.5383
H80	3.535	0.4535	4.578
H81	2.0273	0.5153	2.6308
H82	2.156	-2.1301	-2.3664
H83	3.7485	-3.7061	-3.3531
H84	6.2703	-3.4829	0.1189
H85	-3.0684	-0.5233	-2.1765
H86	-5.3166	-1.0618	-3.0034
H87	-6.4421	-2.6697	0.8213
H88	-5.2751	-2.9501	3.2672
H89	-1.5005	-1.9328	5.0528
H90	-0.6739	-1.0356	2.914
H91	-5.9099	4.1368	0.9745
H92	-3.732	2.3001	4.1934
H93	-2.1341	1.2949	2.61
H94	-1.6355	1.5803	-2.9863

H95	-2.9524	2.7397	-4.7225
H96	-5.6748	4.2653	-1.7666
H97	-2.4494	-4.635	-1.8954
H98	0.2948	-1.3731	-2.4471
H99	-0.6758	-0.9242	-4.6492
H100	-2.5401	-2.3307	-5.5164
H101	-3.423	-4.1866	-4.1057
H102	1.1534	-2.4158	2.1846
H103	1.3435	-4.8376	2.56
H104	0.4816	-6.4228	0.8247
H105	-0.5288	-5.5391	-1.2325
H106	4.6142	5.5747	2.6033
H107	6.3691	2.0936	-3.8974
H108	5.8001	-4.3949	-2.1505
H109	5.6229	-0.8752	4.5453
H110	-3.7628	-2.9204	5.2441
H111	-4.9518	4.0734	-4.1405
H112	-5.617	3.6952	3.4062
H113	-7.0107	-2.1214	-1.5416

4CzBN-ICz S$_0$

C1	0.0847	-1.1312	0.0951
C2	-0.8449	-0.3402	0.8189
C3	-0.9321	1.0483	0.5793
C4	-0.0397	1.6469	-0.3348
C5	0.9822	0.8965	-0.9562
C6	1.0455	-0.4963	-0.7354
C7	-0.1364	3.0525	-0.5999
N8	-0.2189	4.1899	-0.8256
N9	1.937	1.5722	-1.7485
C10	2.8816	2.5025	-1.2721
C11	3.6654	2.9532	-2.3573
C12	3.1616	2.298	-3.5469
C13	2.0957	1.4633	-3.1405
N14	2.1472	-1.2271	-1.2684
C15	2.1774	-2.1659	-2.3149
C16	3.4918	-2.6782	-2.4319
C17	4.2891	-2.048	-1.403

C18	3.4325	-1.17	-0.7021
C19	-2.1021	-1.7618	3.9426
C20	-1.0623	-1.3237	3.0927
N21	-1.6103	-0.9378	1.8539
C22	-3.0083	-1.0932	1.9347
C23	-3.3387	-1.6162	3.2058
C24	-3.5965	3.3581	1.5487
C25	-2.8623	3.2363	2.7915
C26	-1.8095	2.3202	2.5639
N27	-1.8848	1.8638	1.2359
C28	-2.9602	2.5172	0.609
C29	3.4977	2.377	-4.9033
C30	2.7783	1.6447	-5.8478
C31	1.7041	0.8418	-5.4111
C32	1.347	0.743	-4.0696
C33	3.106	2.9671	0.0246
C34	4.1329	3.8858	0.2174
C35	4.9389	4.3507	-0.8432
C36	4.6944	3.8749	-2.1309
C37	5.6265	-2.1734	-1.0085
C38	6.1089	-1.4451	0.0787
C39	5.2231	-0.5931	0.7713
C40	3.8895	-0.445	0.4003
C41	1.1668	-2.6074	-3.1712
C42	1.4897	-3.5553	-4.1373
C43	2.7919	-4.0771	-4.2812
C44	3.7885	-3.6273	-3.4172
C45	-3.9973	-0.8441	0.9837
C46	-5.3178	-1.1047	1.3333
C47	-5.6812	-1.6185	2.5961
C48	-4.6763	-1.8782	3.5262
C49	-1.8045	-2.1866	5.2426
C50	-0.489	-2.1637	5.7057
C51	0.5232	-1.6917	4.8447
C52	0.2576	-1.2687	3.545
C53	-2.9918	3.8393	4.0478
C54	-2.0832	3.5439	5.0643
C55	-1.0343	2.6395	4.797
C56	-0.8794	2.022	3.559

C57	-3.4254	2.4107	-0.7024
C58	-4.5394	3.1646	-1.0589
C59	-5.1993	4.0139	-0.1456
C60	-4.7179	4.1007	1.1606
H61	4.3154	3.0185	-5.2237
H62	1.1322	0.2814	-6.1469
H63	0.5082	0.1262	-3.7671
H64	2.4949	2.6422	0.8609
H65	4.3149	4.2628	1.2212
H66	5.3036	4.224	-2.9615
H67	6.2907	-2.8454	-1.5472
H68	5.5941	-0.0267	1.6224
H69	3.238	0.2256	0.9498
H70	0.151	-2.242	-3.096
H71	0.705	-3.9064	-4.8038
H72	4.8002	-4.0164	-3.5074
H73	-3.7576	-0.4677	-0.0025
H74	-6.0969	-0.9065	0.601
H75	-4.9317	-2.2799	4.5043
H76	-2.6034	-2.524	5.8991
H77	1.5483	-1.6549	5.2068
H78	1.0597	-0.9002	2.9146
H79	-3.7974	4.5468	4.2305
H80	-0.3196	2.4143	5.5853
H81	-0.0632	1.3291	3.3878
H82	-2.9369	1.7675	-1.4282
H83	-4.9108	3.0993	-2.0792
H84	-5.214	4.7504	1.8779
C85	0.087	-2.6061	0.218
C86	1.1664	-3.2087	0.8973
C87	-0.9902	-3.3169	-0.3517
C88	1.1821	-4.6054	1.0217
H89	1.9555	-2.5847	1.306
C90	-1.0001	-4.7152	-0.2422
H91	-1.7809	-2.7718	-0.8581
C92	0.0925	-5.2302	0.4375
C93	1.9629	-5.7232	1.5691
C94	-1.7747	-5.9117	-0.5959
N95	0.0956	-6.592	0.5513

C96	3.163	-5.8054	2.276
C97	1.2584	-6.9386	1.2583
C98	-1.0651	-7.0559	-0.0877
C99	-2.9738	-6.1138	-1.2791
C100	3.6475	-7.0557	2.6617
H101	3.7143	-4.903	2.5234
C102	1.7417	-8.1846	1.6429
C103	-1.5436	-8.3498	-0.261
C104	-3.4533	-7.4124	-1.4526
H105	-3.5274	-5.2661	-1.6719
C106	2.9455	-8.2262	2.3487
H107	4.581	-7.1231	3.2118
H108	1.2041	-9.096	1.4045
C109	-2.7467	-8.512	-0.9502
H110	-1.0032	-9.2076	0.1247
H111	-4.3861	-7.5734	-1.984
H112	3.3422	-9.188	2.6596
H113	-3.1393	-9.5137	-1.0975
H114	3.0332	1.6827	-6.8863
H115	5.7146	5.0632	-0.6547
H116	-6.0499	4.5817	-0.4604
H117	-2.1781	3.9853	6.0343
H118	-6.71	-1.801	2.8266
H119	-0.2441	-2.494	6.6936
H120	3.0003	-4.8042	-5.038
H121	7.1306	-1.5229	0.387

4CzBN S$_1$

C1	0.0234	1.4978	-0.033
C2	-1.1813	0.8206	-0.0864
C3	-1.213	-0.5645	-0.1932
C4	0.0064	-1.3448	-0.284
C5	1.2465	-0.6182	-0.1576
C6	1.2475	0.7539	-0.0364
C7	-0.0422	-2.7224	-0.5106
N8	-0.1653	-3.8712	-0.6988
N9	2.4493	-1.3639	-0.1792
C10	2.8254	-2.3246	0.7599

C11	4.0574	-2.8869	0.3763
C12	4.4353	-2.2541	-0.8698
C13	3.4199	-1.3295	-1.1814
N14	2.4505	1.4973	0.0697
C15	2.8315	2.5069	-0.8126
C16	4.0163	3.1088	-0.3451
C17	4.3559	2.4476	0.8966
C18	3.3652	1.4716	1.1227
C19	-4.0937	2.8031	0.9018
C20	-2.8388	2.2147	1.1616
N21	-2.4052	1.5448	0.0222
C22	-3.3396	1.7494	-0.9893
C23	-4.4131	2.5072	-0.4793
C24	-4.2023	-2.6012	-0.7117
C25	-4.3009	-2.3176	0.7184
C26	-3.1865	-1.5159	1.0383
N27	-2.4455	-1.2753	-0.1201
C28	-3.0319	-1.9396	-1.1642
C29	5.52	-2.4027	-1.7318
C30	5.5729	-1.6378	-2.8862
C31	4.5498	-0.7304	-3.1848
C32	3.4617	-0.564	-2.3419
C33	2.1757	-2.7184	1.9268
C34	2.7855	-3.6871	2.7092
C35	4.0123	-4.2533	2.3443
C36	4.6511	-3.8581	1.1795
C37	5.3836	2.6165	1.8229
C38	5.4036	1.8233	2.9585
C39	4.4021	0.8693	3.1758
C40	3.3713	0.6819	2.2683
C41	2.2239	2.9185	-1.9974
C42	2.8255	3.9466	-2.708
C43	4.0041	4.553	-2.258
C44	4.6029	4.1378	-1.0787
C45	-3.294	1.3541	-2.3231
C46	-4.3649	1.6985	-3.135
C47	-5.4522	2.4265	-2.6379
C48	-5.4784	2.8388	-1.3145
C49	-4.7421	3.512	1.9112

C50	-4.1337	3.6281	3.1514
C51	-2.8809	3.0487	3.3886
C52	-2.2152	2.3364	2.4026
C53	-5.1854	-2.6781	1.7115
C54	-4.9402	-2.2352	3.0205
C55	-3.8306	-1.4549	3.3211
C56	-2.9251	-1.0801	2.3281
C57	-2.5869	-2.0205	-2.4882
C58	-3.3525	-2.771	-3.3685
C59	-4.5124	-3.413	-2.9373
C60	-4.9475	-3.3354	-1.6029
H61	0.0458	2.5748	0.048
H62	6.3096	-3.1113	-1.5022
H63	6.4123	-1.7419	-3.5655
H64	4.6084	-0.1394	-4.0931
H65	2.6766	0.1437	-2.577
H66	1.2177	-2.294	2.204
H67	2.2964	-4.0161	3.6204
H68	4.4627	-5.0102	2.9775
H69	5.6022	-4.2978	0.8956
H70	6.1538	3.3634	1.6571
H71	6.1988	1.9413	3.6869
H72	4.4326	0.2572	4.0713
H73	2.6051	-0.0622	2.4426
H74	1.3076	2.4563	-2.346
H75	2.37	4.287	-3.6325
H76	4.4498	5.3541	-2.8377
H77	5.5177	4.607	-0.7303
H78	-2.4393	0.818	-2.7168
H79	-4.3527	1.4048	-4.1796
H80	-6.2732	2.6813	-3.2993
H81	-6.3122	3.4215	-0.9356
H82	-5.7082	3.9712	1.7265
H83	-4.6255	4.1818	3.9439
H84	-2.4141	3.1676	4.361
H85	-1.231	1.9164	2.5758
H86	-6.0511	-3.2949	1.4957
H87	-5.629	-2.5118	3.8107
H88	-3.6627	-1.1294	4.341

H89	-2.0563	-0.4762	2.5495
H90	-1.6684	-1.5382	-2.7928
H91	-3.0386	-2.8688	-4.4006
H92	-5.0906	-3.9956	-3.6457
H93	-5.8477	-3.8539	-1.2921

4CzBN-BP S$_1$

C1	0.1431	-1.1506	0.1881
C2	-1.0772	-0.4753	0.0525
C3	-1.137	0.8096	-0.4647
C4	0.047	1.5049	-0.9165
C5	1.3004	0.8967	-0.5625
C6	1.3493	-0.3723	-0.0283
C7	-0.0352	2.7267	-1.591
N8	-0.1813	3.7453	-2.1466
N9	2.47	1.6777	-0.7361
C10	2.7683	2.8423	-0.0286
C11	3.9844	3.3689	-0.4958
C12	4.4308	2.5023	-1.5641
C13	3.4688	1.4846	-1.6895
N14	2.5971	-0.8916	0.4267
C15	3.3759	-1.9011	-0.1391
C16	4.485	-2.151	0.6899
C17	4.3625	-1.2709	1.8295
C18	3.1883	-0.523	1.6334
C19	-3.8589	-1.6217	2.1191
C20	-2.5213	-1.2283	1.9279
N21	-2.2779	-1.0587	0.5668
C22	-3.4598	-1.3485	-0.12
C23	-4.4595	-1.6983	0.8057
C24	-4.1568	2.7459	-1.1515
C25	-4.0445	2.9098	0.2968
C26	-2.9069	2.1783	0.6879
N27	-2.3524	1.5568	-0.4303
C28	-3.0795	1.9114	-1.536
C29	5.531	2.5241	-2.4205
C30	5.6688	1.5508	-3.3997
C31	4.6803	0.5574	-3.5129

C32	3.5804	0.5092	-2.6749
C33	2.0552	3.4715	0.9885
C34	2.5905	4.6235	1.5368
C35	3.812	5.1661	1.1005
C36	4.5012	4.5297	0.0779
C37	5.123	-1.0772	2.9826
C38	4.7158	-0.1572	3.9382
C39	3.5289	0.5648	3.722
C40	2.7567	0.3972	2.5853
C41	3.1906	-2.6292	-1.3123
C42	4.1342	-3.5854	-1.6424
C43	5.26	-3.8435	-0.8407
C44	5.4232	-3.1187	0.3296
C45	-3.7138	-1.3706	-1.4878
C46	-4.9909	-1.7089	-1.9038
C47	-6.0164	-2.0391	-1.002
C48	-5.7352	-2.0393	0.3573
C49	-4.3413	-1.8389	3.4084
C50	-3.5057	-1.6596	4.5025
C51	-2.1777	-1.2519	4.283
C52	-1.669	-1.0327	3.0149
C53	-4.7643	3.6089	1.2405
C54	-4.3504	3.5875	2.5852
C55	-3.2081	2.8665	2.9378
C56	-2.466	2.1522	2.0022
C57	-2.8532	1.5608	-2.8707
C58	-3.7339	2.0583	-3.8143
C59	-4.8091	2.8857	-3.4616
C60	-5.017	3.2251	-2.1097
C61	-1.906	-4.149	-2.1586
C62	-0.8544	-3.3438	-1.7055
C63	-0.3637	-2.3705	-2.5849
C64	-0.8853	-2.2276	-3.8653
C65	-1.9196	-3.0487	-4.3015
C66	-2.43	-4.0084	-3.437
C67	0.8067	-2.992	1.7218
C68	0.9317	-4.3236	2.0825
C69	0.4601	-5.3081	1.2263
C70	-0.121	-4.9425	0.0232

C71	-0.257	-3.6026	-0.3614
C72	0.2168	-2.5994	0.5154
H73	6.2778	3.3077	-2.3267
H74	4.7843	-0.2006	-4.2842
H75	2.8325	-0.2657	-2.7838
H76	1.1012	3.0837	1.3269
H77	2.0452	5.1307	2.3279
H78	5.4424	4.9397	-0.2776
H79	6.0332	-1.6503	3.1363
H80	3.2113	1.2857	4.4702
H81	1.8562	0.9795	2.4323
H82	2.3304	-2.4696	-1.9491
H83	3.9979	-4.1612	-2.5537
H84	6.2821	-3.3064	0.9682
H85	-2.9308	-1.1727	-2.2077
H86	-5.1996	-1.736	-2.9696
H87	-6.5085	-2.3103	1.0706
H88	-5.3722	-2.1465	3.5601
H89	-1.5252	-1.1111	5.1402
H90	-0.6389	-0.7308	2.8702
H91	-5.6411	4.1835	0.9584
H92	-2.8888	2.8612	3.9747
H93	-1.5816	1.599	2.2862
H94	-2.0154	0.9338	-3.1445
H95	-3.5859	1.8107	-4.8597
H96	-5.8507	3.866	-1.8417
H97	-2.3347	-4.8861	-1.4887
H98	0.4367	-1.7146	-2.2698
H99	-0.4657	-1.4779	-4.5295
H100	-2.321	-2.9414	-5.3041
H101	-3.248	-4.648	-3.7528
H102	1.1808	-2.2252	2.3907
H103	1.4003	-4.5871	3.0248
H104	0.5579	-6.3578	1.483
H105	-0.4472	-5.7176	-0.6614
H106	4.1923	6.0588	1.5514
H107	6.5093	1.5475	-4.0619
H108	5.9695	-4.5876	-1.1372
H109	5.291	0.0118	4.8245

H110	-6.9898	-2.2939	-1.3659
H111	-3.8542	-1.8338	5.4991
H112	-4.9124	4.1093	3.3314
H113	-5.4556	3.2758	-4.2197

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C1	0.1272	-1.1934	0.1746
C2	-0.8733	-0.3538	0.6801
C3	-1.0449	0.9317	0.1894
C4	-0.2287	1.4603	-0.8843
C5	0.9266	0.6771	-1.2279
C6	1.103	-0.5903	-0.7188
C7	-0.5001	2.7057	-1.456
N8	-0.7786	3.7533	-1.8961
N9	1.8946	1.2881	-2.0641
C10	2.6967	2.3737	-1.7085
C11	3.5099	2.7257	-2.7993
C12	3.1646	1.831	-3.8825
C13	2.1633	0.9715	-3.396
N14	2.3284	-1.2766	-0.9658
C15	2.5574	-2.4026	-1.7582
C16	3.9065	-2.7857	-1.6399
C17	4.5242	-1.8651	-0.7122
C18	3.5218	-0.9626	-0.3166
C19	-2.1187	-1.0756	4.034
C20	-1.089	-0.867	3.0981
N21	-1.6377	-0.7551	1.8212
C22	-3.023	-0.8997	1.9366
C23	-3.3577	-1.0956	3.2889
C24	-3.6583	3.3211	1.0771
C25	-2.7735	3.4375	2.2371
C26	-1.7203	2.5285	2.0182
N27	-1.9368	1.851	0.8207
C28	-3.0794	2.3359	0.2409
C29	3.598	1.7122	-5.2036
C30	3.0353	0.7568	-6.0372
C31	2.0218	-0.0739	-5.5279
C32	1.5744	0.0192	-4.2213

C33	2.7667	3.0734	-0.5065
C34	3.6722	4.1161	-0.4151
C35	4.5074	4.4834	-1.4848
C36	4.4156	3.78	-2.6769
C37	5.8086	-1.7528	-0.1797
C38	6.0936	-0.7586	0.7462
C39	5.0666	0.1189	1.1361
C40	3.7839	0.0333	0.6214
C41	1.6856	-3.131	-2.565
C42	2.188	-4.2209	-3.2536
C43	3.5349	-4.6143	-3.1659
C44	4.3873	-3.8863	-2.3499
C45	-4.0071	-0.9059	0.952
C46	-5.3232	-1.07	1.3498
C47	-5.6897	-1.2445	2.6959
C48	-4.6922	-1.2652	3.66
C49	-1.812	-1.1964	5.3893
C50	-0.4944	-1.101	5.8154
C51	0.513	-0.8734	4.8598
C52	0.2402	-0.754	3.5081
C53	-2.7769	4.2189	3.3709
C54	-1.7238	4.1002	4.2987
C55	-0.6891	3.1956	4.0485
C56	-0.664	2.3979	2.9094
C57	-3.6384	1.9856	-0.993
C58	-4.8002	2.6354	-1.3682
C59	-5.4001	3.6089	-0.5562
C60	-4.815	3.9479	0.6823
H61	4.3728	2.3725	-5.5837
H62	1.5751	-0.8172	-6.1828
H63	0.7906	-0.6313	-3.8547
H64	2.1191	2.8222	0.3258
H65	3.7367	4.6757	0.5144
H66	5.0489	4.0539	-3.5162
H67	6.587	-2.4464	-0.4859
H68	5.2898	0.8964	1.8614
H69	3.0139	0.7317	0.9258
H70	0.6396	-2.8702	-2.6509
H71	1.5144	-4.7959	-3.8835

H72	5.4311	-4.1749	-2.2611
H73	-3.7507	-0.8297	-0.0961
H74	-6.0988	-1.0837	0.589
H75	-4.9504	-1.4178	4.7044
H76	-2.6043	-1.363	6.1138
H77	1.5437	-0.7963	5.1947
H78	1.0348	-0.5918	2.7901
H79	-3.5765	4.929	3.5567
H80	0.1201	3.1118	4.7662
H81	0.1401	1.6992	2.7261
H82	-3.1648	1.246	-1.6242
H83	-5.2578	2.396	-2.3218
H84	-5.2789	4.7084	1.3016
C85	0.1981	-2.6313	0.5179
C86	-0.8175	-3.477	0.0249
C87	1.2767	-3.0662	1.3165
C88	-0.7636	-4.8419	0.342
H89	-1.6128	-3.0577	-0.5841
C90	1.3556	-4.4266	1.649
H91	2.0155	-2.3457	1.6535
C92	0.3229	-5.1899	1.1279
C93	-1.4644	-6.1181	0.1449
C94	2.1652	-5.407	2.3839
N95	0.3873	-6.5178	1.4445
C96	-2.6227	-6.4855	-0.5406
C97	-0.7218	-7.1339	0.8427
C98	1.5345	-6.692	2.2347
C99	3.3366	-5.3168	3.1356
C100	-3.0301	-7.82	-0.5329
H101	-3.2014	-5.7381	-1.0754
C102	-1.1282	-8.4639	0.8501
C103	2.0621	-7.8381	2.8188
C104	3.8653	-6.4673	3.7214
H105	3.8308	-4.3582	3.2626
C106	-2.2921	-8.7927	0.1528
H107	-3.9309	-8.1092	-1.0653
H108	-0.5623	-9.2235	1.3786
C109	3.2354	-7.7079	3.5639
H110	1.5811	-8.8033	2.7021

H111	4.7768	-6.4007	4.3073
H112	-2.6287	-9.825	0.1444
H113	3.6652	-8.5899	4.0293
H114	-6.2933	4.0982	-0.8841
H115	-1.7135	4.6958	5.1875
H116	-6.7191	-1.3698	2.9596
H117	-0.2375	-1.2097	6.8484
H118	3.8832	-5.4624	-3.7176
H119	3.3621	0.6443	-7.0498
H120	5.191	5.2992	-1.3748
H121	7.0762	-0.6482	1.1551

4CzBN T$_1$

C1	0.0242	1.4299	-0.4875
C2	-1.1881	0.7997	-0.3973
C3	-1.2625	-0.6274	-0.3537
C4	0.01	-1.4082	-0.5065
C5	1.2362	-0.7395	-0.3385
C6	1.2623	0.6648	-0.3042
C7	0.0032	-2.8072	-0.6724
N8	0.0065	-3.9664	-0.7975
N9	2.4293	-1.4859	-0.267
C10	2.7557	-2.4083	0.7392
C11	4.1242	-2.7258	0.6379
C12	4.6526	-1.9761	-0.4851
C13	3.5839	-1.2313	-1.018
N14	2.4253	1.3926	-0.0888
C15	2.8941	2.4107	-0.9377
C16	4.1718	2.8147	-0.5045
C17	4.4972	2.0131	0.6623
C18	3.4003	1.1621	0.8943
C19	-4.0014	2.8725	0.6015
C20	-2.6347	2.5292	0.6577
N21	-2.3642	1.5793	-0.3366
C22	-3.5493	1.3331	-1.0379
C23	-4.5856	2.1074	-0.4823
C24	-4.3974	-2.4514	-0.2697
C25	-4.4953	-1.633	0.9284

C26	-3.2765	-0.9422	1.0487
N27	-2.4364	-1.2862	-0.0246
C28	-3.1259	-2.2204	-0.8271
C29	5.9193	-1.8735	-1.0618
C30	6.0949	-1.0338	-2.1529
C31	5.0135	-0.317	-2.6844
C32	3.742	-0.4141	-2.135
C33	1.9602	-2.9147	1.7661
C34	2.5641	-3.7623	2.6859
C35	3.9214	-4.1004	2.5916
C36	4.7069	-3.585	1.5705
C37	5.5929	1.975	1.5206
C38	5.57	1.0935	2.5959
C39	4.4507	0.2867	2.8375
C40	3.3405	0.3228	2.0028
C41	2.3197	2.9176	-2.1026
C42	3.0288	3.8942	-2.7941
C43	4.284	4.3327	-2.3558
C44	4.8675	3.7872	-1.2176
C45	-3.7583	0.5091	-2.1414
C46	-5.0492	0.4253	-2.645
C47	-6.1003	1.1659	-2.0847
C48	-5.8738	2.0181	-1.0131
C49	-4.5289	3.7701	1.5308
C50	-3.6945	4.2994	2.5054
C51	-2.3411	3.9374	2.5565
C52	-1.7902	3.0529	1.6372
C53	-5.4886	-1.4415	1.8837
C54	-5.2425	-0.5688	2.9402
C55	-4.0081	0.0795	3.0653
C56	-2.9973	-0.1135	2.1304
C57	-2.7577	-2.7543	-2.0598
C58	-3.67	-3.5873	-2.6957
C59	-4.9246	-3.8573	-2.1353
C60	-5.3008	-3.2818	-0.9269
H61	0.0714	2.507	-0.5779
H62	6.7527	-2.4416	-0.6596
H63	7.0757	-0.9357	-2.6058
H64	5.167	0.3289	-3.5431

H65	2.9053	0.1319	-2.5579
H66	0.9083	-2.6626	1.845
H67	1.9652	-4.1763	3.4906
H68	4.3573	-4.7721	3.3235
H69	5.7612	-3.835	1.5003
H70	6.4462	2.6248	1.353
H71	6.4213	1.0414	3.2662
H72	4.4432	-0.3828	3.6913
H73	2.4661	-0.2829	2.2089
H74	1.3656	2.5559	-2.4698
H75	2.6017	4.3146	-3.6985
H76	4.8122	5.0932	-2.9207
H77	5.8558	4.1014	-0.8964
H78	-2.9437	-0.0508	-2.5874
H79	-5.2431	-0.2303	-3.488
H80	-7.0975	1.0774	-2.5026
H81	-6.6829	2.6074	-0.5923
H82	-5.5803	4.0394	1.4958
H83	-4.0898	4.9985	3.2346
H84	-1.7042	4.3591	3.3275
H85	-0.7433	2.7745	1.6871
H86	-6.4367	-1.9645	1.8069
H87	-6.0117	-0.3993	3.6862
H88	-3.8312	0.7464	3.9026
H89	-2.0316	0.3682	2.237
H90	-1.7967	-2.5351	-2.5103
H91	-3.4016	-4.0317	-3.6481
H92	-5.6142	-4.511	-2.6587
H93	-6.2869	-3.4608	-0.51

4CzBN-BP T$_1$

C1	0.1684	-1.031	0.1303
C2	-1.106	-0.2622	0.1098
C3	-1.1227	1.0885	-0.2272
C4	0.0942	1.7627	-0.4742
C5	1.3757	1.049	-0.3084
C6	1.3825	-0.3076	-0.0162
C7	0.0929	3.1113	-0.8899

N8	0.092	4.226	-1.2307
N9	2.5462	1.7967	-0.4407
C10	2.904	2.874	0.3917
C11	4.2447	3.2146	0.1459
C12	4.7283	2.3191	-0.8885
C13	3.6604	1.4696	-1.2242
N14	2.6273	-0.9614	0.1614
C15	3.1825	-1.9856	-0.6096
C16	4.4748	-2.2716	-0.1297
C17	4.7084	-1.3974	1.0006
C18	3.546	-0.6196	1.1555
C19	-3.6693	-1.9972	2.0014
C20	-2.3478	-1.5621	1.8151
N21	-2.2487	-0.912	0.5674
C22	-3.519	-0.9224	-0.025
C23	-4.4183	-1.5928	0.8236
C24	-4.1794	2.9221	-0.9843
C25	-4.3465	2.659	0.4303
C26	-3.1785	2.0042	0.8646
N27	-2.3148	1.8477	-0.2216
C28	-2.9181	2.4161	-1.3464
C29	5.9479	2.1898	-1.5511
C30	6.0968	1.2227	-2.5423
C31	4.995	0.4163	-2.8842
C32	3.7674	0.5359	-2.2505
C33	2.1689	3.4958	1.3998
C34	2.7981	4.4961	2.1268
C35	4.1323	4.8765	1.8879
C36	4.854	4.2198	0.8959
C37	5.7817	-1.215	1.8771
C38	5.6934	-0.2718	2.8941
C39	4.5053	0.4714	3.0382
C40	3.4213	0.307	2.19
C41	2.6634	-2.6511	-1.7212
C42	3.4628	-3.5998	-2.3382
C43	4.7601	-3.907	-1.8813
C44	5.2574	-3.2354	-0.7728
C45	-3.9052	-0.4693	-1.2827
C46	-5.2329	-0.6374	-1.6428

C47	-6.1657	-1.2716	-0.8022
C48	-5.7423	-1.7664	0.431
C49	-4.0349	-2.6152	3.1948
C50	-3.0891	-2.7858	4.2039
C51	-1.786	-2.2958	4.0064
C52	-1.4001	-1.668	2.8295
C53	-5.3751	2.911	1.3423
C54	-5.2393	2.5152	2.6672
C55	-4.0482	1.8815	3.0735
C56	-3.006	1.6279	2.1951
C57	-2.4666	2.4541	-2.6649
C58	-3.303	3.0261	-3.6109
C59	-4.5665	3.5556	-3.2799
C60	-4.998	3.4968	-1.9606
C61	-2.6575	-3.4747	-2.0917
C62	-1.4618	-2.8269	-1.7383
C63	-1.0135	-1.7889	-2.5704
C64	-1.7058	-1.4496	-3.7318
C65	-2.8715	-2.1238	-4.0792
C66	-3.3507	-3.132	-3.2446
C67	0.9663	-3.1024	1.2167
C68	0.952	-4.4676	1.4266
C69	0.1149	-5.2755	0.6518
C70	-0.6749	-4.6977	-0.3288
C71	-0.6815	-3.3138	-0.5668
C72	0.146	-2.4899	0.2444
H73	6.7791	2.843	-1.2985
H74	5.1082	-0.327	-3.6689
H75	2.9243	-0.0793	-2.5444
H76	1.1416	3.2166	1.6113
H77	2.2411	5.0043	2.9095
H78	5.8927	4.4824	0.712
H79	6.686	-1.8081	1.764
H80	4.4374	1.2038	3.8387
H81	2.5157	0.8895	2.3227
H82	1.6661	-2.445	-2.0928
H83	3.0735	-4.1298	-3.2038
H84	6.2578	-3.4551	-0.4077
H85	-3.1963	-0.0249	-1.9692

H86	-5.5578	-0.2728	-2.614
H87	-6.442	-2.287	1.0797
H88	-5.0589	-2.9466	3.3465
H89	-1.0581	-2.4006	4.8063
H90	-0.3976	-1.2691	2.7127
H91	-6.2803	3.4173	1.0159
H92	-3.9422	1.5787	4.1123
H93	-2.0946	1.1464	2.5345
H94	-1.4953	2.0539	-2.9395
H95	-2.9713	3.0741	-4.6451
H96	-5.974	3.8916	-1.689
H97	-3.0603	-4.2375	-1.4324
H98	-0.104	-1.2505	-2.3253
H99	-1.3256	-0.6554	-4.3672
H100	-3.409	-1.8581	-4.9838
H101	-4.2783	-3.643	-3.4835
H102	1.5933	-2.471	1.8396
H103	1.5865	-4.9017	2.1921
H104	0.0979	-6.3506	0.7971
H105	-1.2731	-5.3373	-0.969
H106	-6.0204	2.6841	3.3788
H107	-5.1719	3.9998	-4.0422
H108	7.0311	1.0885	-3.0463
H109	4.5736	5.6604	2.4672
H110	5.3399	-4.6508	-2.3868
H111	6.5104	-0.1011	3.5636
H112	-3.3423	-3.2756	5.1209
H113	-7.1822	-1.3763	-1.1194

4CzBN-ICz T$_1$

C1	0.0198	1.4892	-0.2542
C2	-1.0279	0.8531	0.3199
C3	-1.1068	-0.5872	0.3096
C4	-0.0746	-1.3608	-0.4491
C5	1.0725	-0.6967	-0.866
C6	1.1678	0.7045	-0.7453
C7	-0.1457	-2.7651	-0.5749
N8	-0.1976	-3.9249	-0.6775

N9	2.1334	-1.4409	-1.4316
C10	2.9457	-2.3543	-0.758
C11	4.0828	-2.6229	-1.5443
C12	3.9448	-1.8506	-2.7652
C13	2.7346	-1.1429	-2.657
N14	2.308	1.422	-1.1046
C15	2.3453	2.4408	-2.0742
C16	3.6871	2.7627	-2.3496
C17	4.5113	1.9133	-1.5024
C18	3.6289	1.1187	-0.7504
C19	-3.2933	2.6382	2.5364
C20	-1.9938	2.3629	2.0667
N21	-2.0831	1.6063	0.8961
C22	-3.4362	1.4236	0.6012
C23	-4.2192	2.0349	1.5959
C24	-4.1045	-2.3102	1.3982
C25	-3.6764	-1.6466	2.6253
C26	-2.4405	-1.0418	2.3378
N27	-2.1017	-1.2654	0.9972
C28	-3.1073	-2.0735	0.4335
C29	4.7292	-1.6931	-3.9114
C30	4.3077	-0.8466	-4.9291
C31	3.0792	-0.1707	-4.7975
C32	2.2754	-0.3118	-3.6775
C33	2.7784	-2.9201	0.5052
C34	3.7885	-3.7484	0.9718
C35	4.939	-4.0366	0.2133
C36	5.0753	-3.471	-1.049
C37	5.8846	1.7856	-1.3114
C38	6.3682	0.8766	-0.3708
C39	5.4568	0.1353	0.4024
C40	4.0846	0.2568	0.2429
C41	1.2953	3.036	-2.7705
C42	1.6222	3.9908	-3.7252
C43	2.9514	4.3468	-4.0099
C44	3.9846	3.717	-3.3181
C45	-4.0151	0.7781	-0.4903
C46	-5.3976	0.7012	-0.5294
C47	-6.2105	1.2747	0.4681

C48	-5.6129	1.9558	1.5213
C49	-3.4626	3.3421	3.7305
C50	-2.3508	3.7614	4.4518
C51	-1.0652	3.4713	3.9551
C52	-0.8636	2.7826	2.7684
C53	-4.2119	-1.5295	3.901
C54	-3.5065	-0.829	4.8849
C55	-2.2465	-0.2881	4.5807
C56	-1.687	-0.3982	3.3152
C57	-3.2511	-2.4913	-0.8868
C58	-4.4022	-3.1977	-1.2095
C59	-5.4046	-3.4704	-0.2642
C60	-5.2513	-3.0104	1.0456
H61	5.6691	-2.2306	-4.0096
H62	2.752	0.4819	-5.6034
H63	1.326	0.2075	-3.5933
H64	1.8932	-2.7194	1.0996
H65	3.6843	-4.2051	1.9528
H66	5.9595	-3.682	-1.6456
H67	6.5789	2.3895	-1.8896
H68	5.8397	-0.5564	1.1482
H69	3.3942	-0.3083	0.8576
H70	0.2634	2.7583	-2.5859
H71	0.822	4.4769	-4.2772
H72	5.0194	3.9608	-3.5438
H73	-3.4027	0.3333	-1.2677
H74	-5.8728	0.1775	-1.3551
H75	-6.2289	2.4175	2.2891
H76	-4.4633	3.5535	4.0995
H77	-0.1995	3.8062	4.5213
H78	0.1354	2.5693	2.4032
H79	-5.1706	-1.9799	4.1424
H80	-1.6974	0.2336	5.3599
H81	-0.7049	0.002	3.0903
H82	-2.4957	-2.2775	-1.6335
H83	-4.535	-3.5517	-2.2277
H84	-6.0362	-3.186	1.7764
C85	0.0818	2.9676	-0.2838
C86	1.2485	3.5879	0.21

C87	-1.0294	3.664	-0.8039
C88	1.3217	4.9881	0.1883
H89	2.0583	2.9743	0.5932
C90	-0.9833	5.0654	-0.8377
H91	-1.8884	3.1057	-1.1634
C92	0.1937	5.598	-0.3359
C93	2.1931	6.1203	0.5313
C94	-1.7551	6.2532	-1.2257
N95	0.2519	6.9631	-0.3626
C96	3.4665	6.2207	1.0925
C97	1.4966	7.328	0.1756
C98	-0.9579	7.4107	-0.9165
C99	-3.0163	6.4377	-1.792
C100	4.0298	7.4812	1.2938
H101	4.0136	5.3244	1.3698
C102	2.0584	8.5841	0.3764
C103	-1.4126	8.7005	-1.1674
C104	-3.4719	7.7321	-2.0435
H105	-3.6364	5.5797	-2.0341
C106	3.3342	8.6439	0.9401
H107	5.0205	7.5628	1.7303
H108	1.5264	9.4897	0.1052
C109	-2.68	8.8449	-1.7347
H110	-0.8062	9.5683	-0.9317
H111	-4.453	7.8795	-2.484
H112	3.7931	9.614	1.1061
H113	-3.0556	9.8431	-1.9391
H114	5.6843	-4.6955	0.6072
H115	-6.2725	-4.0255	-0.5533
H116	-3.9116	-0.7015	5.867
H117	-7.2741	1.1775	0.4027
H118	-2.4556	4.3014	5.3696
H119	3.1561	5.0863	-4.7557
H120	4.9002	-0.6987	-5.8077
H121	7.4194	0.7383	-0.2262

4CzBN-ICz S$_2$

C1	0.1431	-1.1506	0.1881

C2	-0.311	-0.1976	1.1095
C3	-0.5817	1.1065	0.7244
C4	-0.4389	1.5411	-0.6468
C5	0.2386	0.6256	-1.5237
C6	0.5236	-0.662	-1.125
C7	-0.8725	2.8035	-1.0627
N8	-1.2564	3.8736	-1.3368
N9	0.6453	1.1215	-2.7873
C10	1.6041	2.1147	-2.9877
C11	1.7153	2.3799	-4.3631
C12	0.752	1.5322	-5.0301
C13	0.1071	0.7852	-4.0287
N14	1.3068	-1.4993	-1.973
C15	0.8997	-2.6087	-2.7141
C16	2.0208	-3.1863	-3.3382
C17	3.1705	-2.4082	-2.9368
C18	2.6906	-1.3903	-2.0941
C19	0.3568	-0.8377	4.6404
C20	0.7415	-0.7548	3.2892
N21	-0.3833	-0.5256	2.5002
C22	-1.4951	-0.466	3.3444
C23	-1.0771	-0.6523	4.6746
C24	-1.9802	3.7531	2.8171
C25	-0.587	3.755	3.2599
C26	0.0605	2.744	2.5244
N27	-0.8661	2.1127	1.6956
C28	-2.0815	2.7265	1.8473
C29	0.377	1.3713	-6.3635
C30	-0.6368	0.4849	-6.6982
C31	-1.276	-0.2334	-5.6725
C32	-0.9224	-0.0964	-4.3418
C33	2.3815	2.8	-2.0576
C34	3.2796	3.7394	-2.532
C35	3.4237	4.0161	-3.903
C36	2.6314	3.3299	-4.8123
C37	4.537	-2.5036	-3.1997
C38	5.4211	-1.6033	-2.6223
C39	4.9136	-0.6057	-1.7714
C40	3.5624	-0.4838	-1.4962

C41	-0.3671	-3.1642	-2.8794
C42	-0.489	-4.282	-3.6852
C43	0.6118	-4.869	-4.3337
C44	1.8673	-4.3113	-4.149
C45	-2.842	-0.3046	3.0352
C46	-3.7499	-0.2938	4.0812
C47	-3.3597	-0.4529	5.4216
C48	-2.0144	-0.6415	5.707
C49	1.3201	-1.0503	5.6249
C50	2.6577	-1.1719	5.2738
C51	3.0156	-1.0703	3.9174
C52	2.0816	-0.864	2.9173
C53	0.1329	4.5162	4.1542
C54	1.5099	4.2771	4.3184
C55	2.1257	3.2787	3.5614
C56	1.4187	2.4968	2.653
C57	-3.2792	2.4539	1.1788
C58	-4.3779	3.2276	1.5068
C59	-4.3061	4.2498	2.4634
C60	-3.088	4.5056	3.1243
H61	0.8733	1.9452	-7.1412
H62	-2.0747	-0.9221	-5.9335
H63	-1.4314	-0.6604	-3.5707
H64	2.273	2.619	-0.9943
H65	3.8907	4.2875	-1.8202
H66	2.7234	3.537	-5.8749
H67	4.9116	-3.2863	-3.8535
H68	5.6063	0.0994	-1.3205
H69	3.1936	0.3055	-0.8525
H70	-1.2368	-2.7499	-2.3867
H71	-1.4721	-4.7251	-3.8187
H72	2.7333	-4.7526	-4.6347
H73	-3.1781	-0.2327	2.0092
H74	-4.8051	-0.1749	3.8518
H75	-1.6936	-0.7858	6.7349
H76	1.0267	-1.1188	6.6687
H77	4.0628	-1.1648	3.6441
H78	2.3801	-0.8014	1.8779
H79	-0.3465	5.3041	4.7268

H80	3.1894	3.1051	3.6859
H81	1.9063	1.7277	2.0704
H82	-3.3312	1.6745	0.4306
H83	-5.322	3.0471	1.0046
H84	-3.0374	5.298	3.864
H85	4.1309	4.7499	-4.2291
H86	-0.9339	0.3433	-7.7162
H87	0.4716	-5.7294	-4.9541
H88	6.4715	-1.6549	-2.8196
H89	-4.0938	-0.4376	6.1998
H90	3.4101	-1.348	6.0138
H91	2.0764	4.8473	5.0247
H92	-5.1682	4.8477	2.6738
C93	0.2194	-2.6509	0.527
C94	-1.0034	-3.3313	0.7
C95	1.5057	-3.2182	0.6358
C96	-0.9387	-4.7319	1.0163
H97	-1.9499	-2.8041	0.5949
C98	1.5816	-4.6182	0.9519
H99	2.3947	-2.6088	0.4844
C100	0.3485	-5.2086	1.1046
C101	-1.7573	-5.8953	1.2922
C102	2.5143	-5.7019	1.1834
N103	0.419	-6.5939	1.4173
C104	-3.1383	-6.1282	1.3662
C105	-0.8698	-7.0467	1.5392
C106	1.7481	-6.9274	1.473
C107	3.9126	-5.8085	1.1863
C108	-3.6065	-7.4105	1.6634
H109	-3.8409	-5.3132	1.1927
C110	-1.3558	-8.33	1.8365
C111	2.3624	-8.1599	1.744
C112	4.5091	-7.0423	1.4576
H113	4.5285	-4.9332	0.9781
C114	-2.7337	-8.5061	1.8975
H115	-4.6837	-7.5787	1.7182
H116	-0.6724	-9.1605	2.0137
C117	3.7517	-8.2112	1.7348
H118	1.7659	-9.0478	1.9548

H119	5.5983	-7.1129	1.4569
H120	-3.1478	-9.487	2.1254
H121	4.2629	-9.1502	1.9407

4CzBN T$_2$

C1	0.0022	1.3664	-0.1778
C2	-1.2208	0.6913	-0.1778
C3	-1.2324	-0.7112	-0.0127
C4	0.0044	-1.3798	0.158
C5	1.24	-0.6877	0.1622
C6	1.2262	0.7132	-0.0154
C7	0.0056	-2.8029	0.3321
N8	0.0066	-3.9567	0.4731
N9	2.4428	-1.403	0.3438
C10	2.8243	-2.0943	1.5095
C11	4.0993	-2.6699	1.2985
C12	4.5016	-2.3323	-0.052
C13	3.4623	-1.5532	-0.6137
C14	-3.9428	3.118	0.05
C15	-2.7728	2.499	0.5528
N16	-2.4065	1.4517	-0.3098
C17	-3.3119	1.4284	-1.3855
C18	-4.2822	2.4406	-1.1845
C19	-4.0881	-2.9135	-0.6372
C20	-4.4912	-2.2609	0.5923
C21	-3.4532	-1.3678	0.9496
N22	-2.4338	-1.4511	-0.0163
C23	-2.8139	-2.4035	-0.9809
C24	5.6272	-2.6365	-0.8253
C25	5.6958	-2.1697	-2.135
C26	4.6477	-1.4095	-2.6789
C27	3.5154	-1.0944	-1.9294
C28	2.1516	-2.2227	2.7256
C29	2.7766	-2.9494	3.7378
C30	4.04	-3.5311	3.5456
C31	4.7056	-3.3944	2.3305
C32	-3.3156	0.6277	-2.5274
C33	-4.3315	0.8329	-3.4593

C34	-5.315	1.8167	-3.2664
C35	-5.2932	2.6257	-2.1342
C36	-4.5169	4.1806	0.7564
C37	-3.9223	4.6098	1.94
C38	-2.762	3.9843	2.4242
C39	-2.1723	2.9212	1.7411
C40	-5.6165	-2.3717	1.4164
C41	-5.686	-1.6031	2.575
C42	-4.6392	-0.7326	2.9194
C43	-3.5074	-0.6056	2.1159
C44	-2.1409	-2.8203	-2.1302
C45	-2.7645	-3.7705	-2.9375
C46	-4.0271	-4.2906	-2.6105
C47	-4.693	-3.8662	-1.464
H48	0.0013	2.4429	-0.3095
H49	6.4334	-3.2348	-0.4094
H50	6.5646	-2.399	-2.7451
H51	4.7161	-1.0577	-3.7044
H52	2.7109	-0.5099	-2.3622
H53	1.1697	-1.7872	2.8819
H54	2.2692	-3.071	4.6907
H55	4.4995	-4.0942	4.3527
H56	5.6846	-3.8427	2.1842
H57	-2.5644	-0.1358	-2.6916
H58	-4.3591	0.2141	-4.3517
H59	-6.0948	1.9493	-4.0107
H60	-6.0455	3.3969	-1.9917
H61	-5.4161	4.6642	0.3844
H62	-4.3579	5.4356	2.4947
H63	-2.3106	4.333	3.3488
H64	-1.2742	2.4467	2.1243
H65	-6.4216	-3.0539	1.1571
H66	-6.5547	-1.68	3.2226
H67	-4.7084	-0.1442	3.8299
H68	-2.7038	0.0672	2.3949
H69	-1.1596	-2.4336	-2.3872
H70	-2.2568	-4.1174	-3.833
H71	-4.4855	-5.0325	-3.258
H72	-5.6713	-4.2677	-1.2138

N73	2.4568	1.5151	-0.0729
C74	2.8703	2.2537	-1.1697
C75	3.3693	1.6406	0.9621
C76	4.1304	2.8898	-0.8036
C77	2.2926	2.422	-2.394
C78	3.371	1.097	2.2132
C79	4.4327	2.5185	0.4875
C80	4.7903	3.7334	-1.7844
C81	2.9764	3.2645	-3.3376
H82	1.3554	1.9446	-2.6564
C83	4.4771	1.4208	3.0733
H84	2.5757	0.4454	2.5566
C85	5.5325	2.8216	1.3862
C86	4.1952	3.8937	-3.0154
H87	5.7278	4.2182	-1.5386
H88	2.5396	3.4155	-4.3178
C89	5.5203	2.2656	2.6456
H90	4.5037	1.0025	4.0727
H91	6.3359	3.4712	1.059
H92	4.6718	4.52	-3.763
H93	6.3329	2.4793	3.333

4CzBN-BP T$_2$

C1	0.1047	-1.113	0.111
C2	-1.1497	-0.4503	0.1129
C3	-1.2194	0.9362	-0.1449
C4	-0.0248	1.662	-0.3359
C5	1.2366	1.0418	-0.2014
C6	1.299	-0.3494	0.0291
C7	-0.0884	3.0659	-0.6191
N8	-0.1366	4.2027	-0.8575
N9	2.399	1.8427	-0.2607
C10	2.7633	2.8251	0.6808
C11	3.99	3.4034	0.2853
C12	4.3747	2.7736	-0.9611
C13	3.3732	1.8265	-1.2734
N14	2.5666	-0.948	0.2869
C15	3.3279	-1.8177	-0.5142

C16	4.4881	-2.2	0.2012
C17	4.4218	-1.5605	1.4966
C18	3.227	-0.8067	1.5197
C19	-3.8397	-2.2278	1.8352
C20	-2.5433	-1.6698	1.7729
N21	-2.3178	-1.1699	0.4758
C22	-3.4914	-1.377	-0.2757
C23	-4.4415	-2.0423	0.5326
C24	-4.1619	2.9253	-1.0179
C25	-4.3214	2.7994	0.4163
C26	-3.2503	2.0047	0.8851
N27	-2.4537	1.6256	-0.2099
C28	-2.9963	2.2087	-1.3684
C29	5.4492	2.9568	-1.8393
C30	5.5243	2.2173	-3.0194
C31	4.4948	1.2984	-3.3125
C32	3.415	1.0944	-2.4589
C33	2.1122	3.2355	1.8449
C34	2.7133	4.2299	2.6101
C35	3.9413	4.8226	2.2477
C36	4.5723	4.3991	1.0786
C37	5.2464	-1.5872	2.6275
C38	4.8854	-0.8831	3.7762
C39	3.6756	-0.1577	3.7752
C40	2.8371	-0.1095	2.6649
C41	3.1007	-2.3007	-1.8044
C42	4.0441	-3.1578	-2.3623
C43	5.2124	-3.5486	-1.6759
C44	5.4228	-3.0596	-0.3881
C45	-3.7779	-1.0589	-1.6029
C46	-5.033	-1.3967	-2.0974
C47	-6.006	-2.0529	-1.3142
C48	-5.6939	-2.3784	0.0045
C49	-4.3022	-2.7783	3.0359
C50	-3.4941	-2.7644	4.1729
C51	-2.2172	-2.1722	4.0882
C52	-1.7288	-1.622	2.9059
C53	-5.2528	3.3087	1.3288
C54	-5.1177	3.0414	2.691

C55	-4.0274	2.2587	3.1258
C56	-3.086	1.7365	2.2437
C57	-2.5574	2.1379	-2.6913
C58	-3.3054	2.8011	-3.6594
C59	-4.4744	3.5258	-3.3442
C60	-4.8951	3.5789	-2.0155
H61	6.2234	3.6841	-1.606
H62	4.5441	0.7297	-4.2382
H63	2.6338	0.3886	-2.7181
H64	1.159	2.8117	2.1451
H65	2.2139	4.5655	3.5161
H66	5.5179	4.8466	0.7813
H67	6.1687	-2.1634	2.6136
H68	3.3878	0.3882	4.6708
H69	1.9177	0.4649	2.6956
H70	2.2162	-2.0354	-2.3687
H71	3.8696	-3.5408	-3.3654
H72	6.3153	-3.3486	0.1624
H73	-3.0522	-0.5723	-2.2419
H74	-5.2683	-1.1463	-3.1292
H75	-6.4257	-2.8896	0.626
H76	-5.3003	-3.2076	3.0867
H77	-1.5903	-2.1419	4.9766
H78	-0.7459	-1.1637	2.8806
H79	-6.0794	3.9216	0.9768
H80	-3.9171	2.0534	4.1881
H81	-2.2618	1.1352	2.6108
H82	-1.6604	1.5901	-2.9641
H83	-2.9734	2.7626	-4.6945
H84	-5.7937	4.1329	-1.7543
C85	0.1914	-2.6462	0.2266
C86	-0.0993	-3.4695	-0.9506
C87	0.537	-3.2052	1.4226
C88	-0.4523	-2.9172	-2.1748
C89	0.0088	-4.9165	-0.745
C90	0.6293	-4.6095	1.5763
H91	0.7441	-2.5633	2.2688
C92	-0.5596	-1.4701	-2.3808
C93	-0.7437	-3.7405	-3.3518

C94	0.3569	-5.443	0.4649
H95	-0.1898	-5.5881	-1.565
H96	0.9037	-5.0387	2.5278
C97	-0.9078	-0.9437	-3.5907
H98	-0.3598	-0.7985	-1.5611
C99	-1.0892	-3.1816	-4.5479
H100	-0.6861	-4.8149	-3.2787
H101	0.426	-6.5171	0.5768
C102	-1.1809	-1.7773	-4.7018
H103	-0.9763	0.1304	-3.7027
H104	-1.2969	-3.8236	-5.3939
H105	-1.4552	-1.3481	-5.6534
H106	-5.019	4.0266	-4.1172
H107	-5.823	3.4199	3.4011
H108	-6.9619	-2.2905	-1.7321
H109	-3.8286	-3.1935	5.0942
H110	5.9147	-4.2089	-2.1403
H111	5.5108	-0.8838	4.6444
H112	6.344	2.3387	-3.6964
H113	4.3681	5.5893	2.86

4CzBN-ICz T$_2$

C1	0.1047	-1.113	0.111
C2	-0.9243	-0.3883	0.7657
C3	-1.0789	0.9949	0.528
C4	-0.1587	1.6562	-0.3124
C5	0.9518	0.9762	-0.8584
C6	1.0853	-0.4119	-0.6394
C7	-0.3215	3.056	-0.5755
N8	-0.4555	4.1892	-0.798
N9	1.9192	1.7165	-1.5741
C10	2.7687	2.6968	-1.0248
C11	3.5997	3.2054	-2.0477
C12	3.223	2.534	-3.2747
C13	2.1834	1.6327	-2.9518
N14	2.2689	-1.0684	-1.0863
C15	2.4427	-1.9899	-2.1343
C16	3.7925	-2.4165	-2.1485

C17	4.463	-1.7505	-1.0538
C18	3.4983	-0.9374	-0.4176
C19	-2.2971	-1.9964	3.7476
C20	-1.2268	-1.5053	2.967
N21	-1.7285	-1.0416	1.7356
C22	-3.1279	-1.2036	1.7521
C23	-3.505	-1.8052	2.9745
C24	-3.9568	3.1124	1.3095
C25	-3.3132	3.0214	2.604
C26	-2.1857	2.1828	2.4492
N27	-2.1267	1.744	1.1146
C28	-3.1938	2.3318	0.4131
C29	3.6509	2.6468	-4.6027
C30	3.0474	1.8826	-5.6012
C31	1.9957	1.0111	-5.2481
C32	1.5493	0.8775	-3.937
C33	2.8703	3.1609	0.2873
C34	3.8225	4.138	0.5596
C35	4.6731	4.6616	-0.4369
C36	4.5516	4.1853	-1.7418
C37	5.7692	-1.7974	-0.5526
C38	6.1148	-1.0548	0.5765
C39	5.1236	-0.2698	1.2018
C40	3.8177	-0.2004	0.7245
C41	1.5341	-2.4848	-3.0718
C42	1.9934	-3.3984	-4.0154
C43	3.3339	-3.8344	-4.0579
C44	4.2273	-3.3327	-3.1135
C45	-4.0808	-0.8963	0.7814
C46	-5.4128	-1.1799	1.0632
C47	-5.8224	-1.7718	2.2767
C48	-4.853	-2.0879	3.2267
C49	-2.0482	-2.5005	5.0292
C50	-0.7512	-2.506	5.5428
C51	0.2916	-1.9802	4.7526
C52	0.0744	-1.4773	3.4723
C53	-3.5805	3.5936	3.8533
C54	-2.7337	3.3453	4.9334
C55	-1.6082	2.5171	4.7391

C56	-1.3165	1.9321	3.5105
C57	-3.5489	2.2145	-0.9315
C58	-4.6819	2.8962	-1.3652
C59	-5.4667	3.6844	-0.4968
C60	-5.0938	3.7832	0.8435
H61	4.45	3.3385	-4.859
H62	1.5146	0.4235	-6.0266
H63	0.7309	0.207	-3.6996
H64	2.2215	2.7911	1.0751
H65	3.9083	4.515	1.5762
H66	5.1963	4.5792	-2.524
H67	6.5161	-2.4193	-1.0406
H68	5.3877	0.3064	2.0857
H69	3.0823	0.4199	1.2251
H70	0.494	-2.1861	-3.0757
H71	1.2886	-3.7908	-4.7451
H72	5.2659	-3.6558	-3.1245
H73	-3.8052	-0.4586	-0.1696
H74	-6.164	-0.9372	0.3153
H75	-5.144	-2.5501	4.1673
H76	-2.8706	-2.8783	5.6325
H77	1.3019	-1.9649	5.1555
H78	0.8989	-1.0694	2.8974
H79	-4.4453	4.2405	3.981
H80	-0.9437	2.3264	5.5787
H81	-0.445	1.2972	3.3962
H82	-2.9633	1.6175	-1.6241
H83	-4.9688	2.8219	-2.4118
H84	-5.6869	4.3863	1.5269
H85	-6.3282	4.1974	-0.8705
H86	-2.9259	3.7718	5.8958
H87	-6.8587	-1.9689	2.4559
H88	-0.5433	-2.9006	6.5154
H89	3.6484	-4.5376	-4.8005
H90	7.1118	-1.0707	0.9646
H91	3.3694	1.9501	-6.6194
H92	5.3888	5.4172	-0.1883
C93	0.1914	-2.6462	0.2266
C94	-0.8268	-3.3964	-0.3786

C95	1.2805	-3.1785	0.9277
C96	-0.7624	-4.8696	-0.2793
H97	-1.6339	-2.8991	-0.9023
C98	1.3813	-4.6486	1.0496
H99	2.023	-2.5224	1.3646
C100	0.3397	-5.3135	0.4263
C101	-1.4479	-6.0536	-0.6594
C102	2.1902	-5.677	1.5959
N103	0.4162	-6.6694	0.5286
C104	-2.6306	-6.3167	-1.3869
C105	-0.6951	-7.1909	-0.1438
C106	1.5733	-6.9568	1.2622
C107	3.3897	-5.6944	2.3452
C108	-3.0286	-7.6264	-1.5824
H109	-3.2152	-5.4935	-1.7847
C110	-1.1021	-8.4928	-0.3455
C111	2.1217	-8.1593	1.6529
C112	3.9296	-6.9071	2.7309
H113	3.875	-4.7608	2.6105
C114	-2.2808	-8.7038	-1.0725
H115	-3.9359	-7.8324	-2.1404
H116	-0.531	-9.3279	0.0445
C117	3.3113	-8.1255	2.3939
H118	1.6514	-9.1021	1.3972
H119	4.8496	-6.9248	3.3057
H120	-2.6214	-9.7189	-1.2442
H121	3.7617	-9.059	2.7127

Reference

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