# Unraveling Emission Narrowing Pathways in *N*-Embedded Polyaromatic Systems *via* Sequential π-Interlocking for Efficient Electroluminescence

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**Supplementary Information**

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## Experimental Details

### General methods

All solvents and reagents were used as received from commercial suppliers without further purification. The intermediates were synthesized following previously reported procedures.[1] All reactions were conducted under an inert atmosphere. The structure of the target compound was confirmed by nuclear magnetic resonance spectroscopy ($^{1}$H and $^{13}$C NMR). The photophysical properties of the target compound were investigated using UV-visible absorption and fluorescence spectroscopy with freshly prepared solutions. Thermal stability was evaluated via thermogravimetric analysis (TGA) under an inert atmosphere at a heating rate of 10 °C/min. Electrochemical properties were examined using a standard three electrode setup consisting of a silver reference electrode, a carbon working electrode, and a platinum counter electrode; ferrocene used as an internal standard. For theoretical insights, density functional theory (DFT) calculations were performed using the B3LYP functional and

the 6-31G(d,p) basis set. Fluorescence lifetime decay measurements were recorded in a 1 cm quartz cell on a Horiba Jobin Yvon "FluoroCube Fluorescence Lifetime System" equipped with NanoLEDs and LDs as the excitation source(s) and an automated polarization accessory (Model 5000 U-02). The hole only (HOD) and electron only (EOD) devices were fabricated using the configuration: for HOD device: PEDOT(40 nm)/TAPC(10 nm)/CzCz or CzICz (30 nm)/TAPC(20 nm)/Al(200 nm) and for EOD device: PEDOT(40 nm)/TSPO1(20 nm)/CzCz or CzICz (30 nm)/TSPO1(10 nm)/LiF(1.5 nm)/Al(200 nm)

**Synthesis**

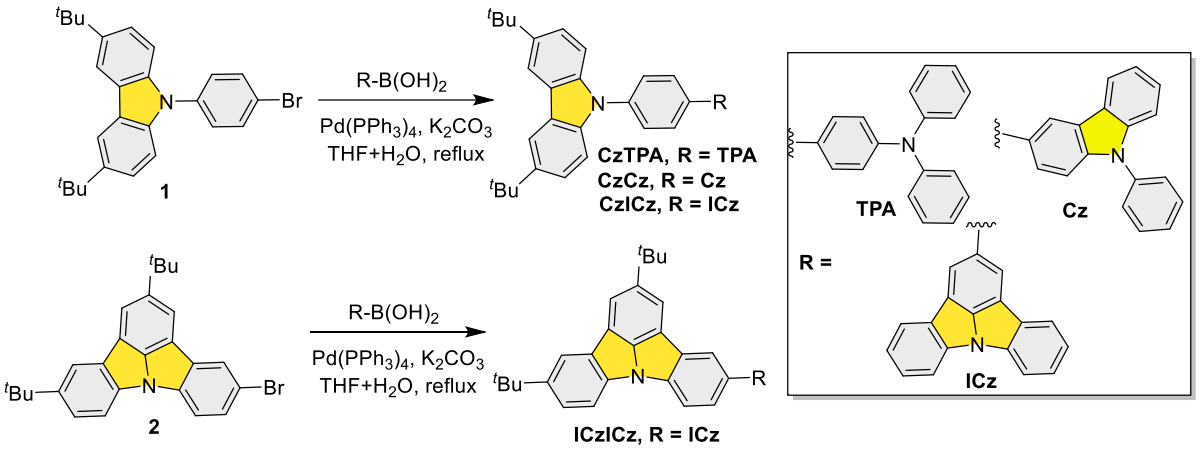
**Synthesis of (4'-(3,6-di-*tert*-butyl-9*H*-carbazol-9-yl)-N,N-diphenyl-[1,1'-biphenyl]-4-amine) CzTPA**: In a 250 mL two neck round-bottomed flask, the mixture of 9-(4-bromophenyl)-3,6-di-*tert*-butyl-9*H*-carbazole **1** (0.3 g, 0.69 mmol), (4-(diphenylamino)phenyl)boronic acid (0.22 g, 0.76 mmol) and potassium carbonate (0.477 g, 3.45 mmol) were dissolved in tetrahydrofuran (20 mL) and water (5 mL) in inert atmosphere, the $Pd(PPh_3)_4$ (40 mg, 0.034 mmol) was added to it. The resulting mixture was refluxed at 80 ºC for 12 h under a nitrogen atmosphere. The mixture was cooled and the solvent was evaporated to dryness. The residue was subjected to column chromatography on silica (cyclohexane: dichloromethane (9:1)) to give the desired product **CzTPA** as a white solid with 70% yield (0.28 g). $^1$H NMR (400.25 MHz, $CDCl_3$, δ ppm): 8.00-7.98 (m, 2H), 7.77-7.73 (m, 2H), 7.61-7.55 (m, 8H), 6.92-6.89 (m, 3H), 6.88-66 (m, 3H), 1.32 (s, 18H); $^{13}$C{1H} NMR (400 MHz, $CDCl_3$, δ ppm): 147.74, 147.65, 147.47, 142.85, 139.25, 136.88, 134.11, 129.36, 129.27, 127.83, 127.75, 127.32, 126.94, 124.56, 124.32, 124.10, 123.85, 123.62, 123.39, 123.10, 122.84, 116.25, 109.30, 34.76, 32.06.

**(3,6-di-*tert*-butyl-9-(4-(9-phenyl-9*H*-carbazol-3-yl)phenyl)-9*H*-carbazole) CzCz:** The **CzCz** was synthesized employing the same synthetic procedure as **CzTPA** using **1** (0.3 g, 0.69 mmol), (9-phenyl-9*H*-carbazol-3-yl)boronic acid (0.218 g, 0.76 mmol), potassium carbonate

(0.477 g, 3.45 mmol) and $Pd(PPh_3)_4$ (40 mg, 0.034 mmol). White solid with 65% yield (0.27 g). $^1H$ NMR (400.25 MHz, $CDCl_3$, δ ppm): 8.36 (s, 2H), 8.23-818 (m, 4H), 7.99-7.95 (m, 5H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.66-7.59 (m, 2H), 7.53-7.50 (m, 5H), 7.49-7.39 (m, 2H), 1.49 (s, 18H); $^{13}C\{1H\}$ NMR (400 MHz, $CDCl_3$, δ ppm): 143.81, 142.95, 142.17, 139.44, 139.35, 136.90, 130.19, 129.57, 127.14, 123.73, 123.51, 123.40, 122.03, 119.35, 118.88, 116.36, 112.47, 109.41, 34.85, 32.14.

**(2-(4-(3,6-di-*tert*-butyl-9*H*-carbazol-9-yl)phenyl)indolo[3,2,1-jk]carbazole) CzICz:** The **CzICz** was synthesized employing the same synthetic procedure as **CzTPA** using **1** (0.3 g, 0.69 mmol), (9-phenyl-9*H*-carbazol-3-yl)boronic acid (0.218 g, 0.76 mmol), potassium carbonate (0.477 g, 3.45 mmol) and $Pd(PPh_3)_4$ (40 mg, 0.034 mmol). White solid with 70% yield (0.26 g). $^1H$ NMR (400.25 MHz, $CDCl_3$, δ ppm): 8.46 (s, 1H), 8.24-8.18 (m, 3H), 7.94-7.91 (m, 2H), 7.67-7.63 (m, 2H), 7.52-7.50 (m, 4H), 7.50-7.45 (m, 6H), 7.36-7.32 (m, 2H), 1.49 (s, 18H); $^{13}C\{1H\}$ NMR (400 MHz, $CDCl_3$, δ ppm): 142.91, 141.53, 140.74, 140.63, 139.43, 137.73, 136.79, 132.69, 130.06, 128.58, 127.70, 127.21, 127.12, 126.36, 125.48, 124.10, 123.70, 123.55, 123.48, 120.50, 120.28, 118.93, 116.33, 110.29, 110.10, 109.41, 34.84, 32.14.

**(2',11'-di-*tert*-butyl-2,5'-biindolo[3,2,1-jk]carbazole) ICzICz:** The **ICzICz** was synthesized employing the same synthetic procedure as **CzTPA** using **2** (0.3 g, 0.81 mmol), indolo[3,2,1-jk]carbazol-2-yl boronic acid (0.254 g, 0.89 mmol), potassium carbonate (0.337 g, 2.44 mmol) and $Pd(PPh_3)_4$ (47 mg, 0.040 mmol). White solid with 77% yield (0.31 g). $^1H$ NMR (400.25 MHz, $CDCl_3$, δ ppm): 8.55 (s, 1H), 8.43-8.41(m, 2H), 8.26-8.13 (m, 5H), 8.01-7.88 (m, 5H), 7.66-7.59 (m, 3H), 7.44-7.40 (m, 2H); $^{13}C\{1H\}$ NMR (400 MHz, $CDCl_3$, δ ppm): 142.93, 139.34, 130.17, 127.10, 122.02, 119.34, 116.34, 112.46, 109.38, 34.84, 32.12.




**Scheme S1**. Synthetic pathway for **CzTPA, CzCz, CzICz** and **ICzICz**

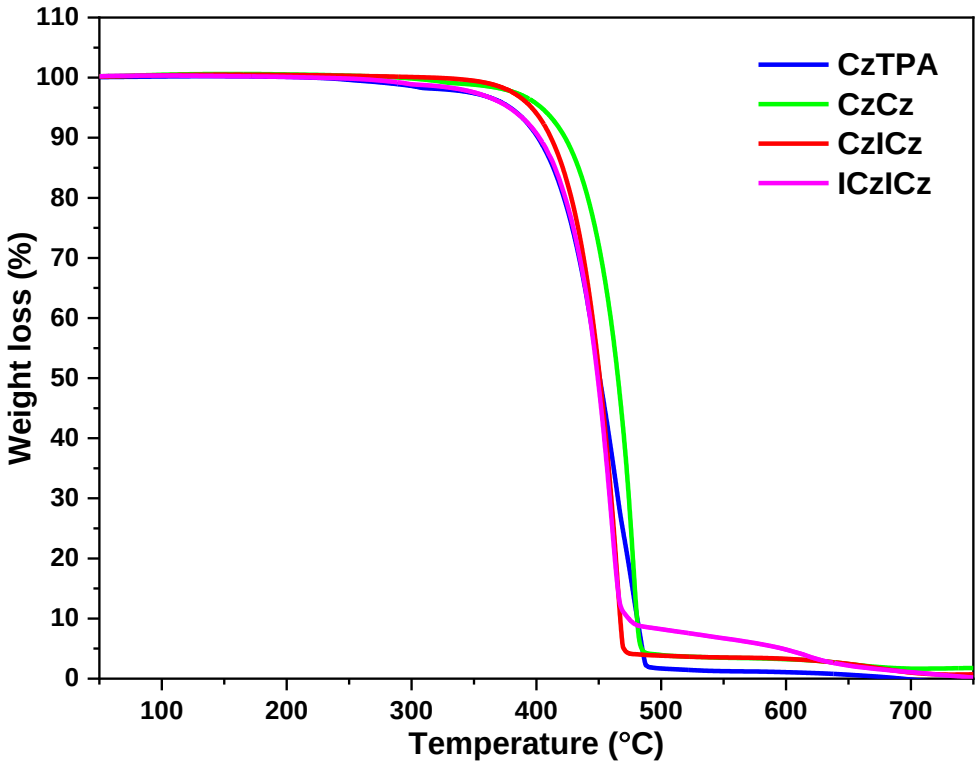



**Figure S1.** TGA plot of the compounds **CzTPA**, **CzCz**, **CzICz** and **ICzICz**

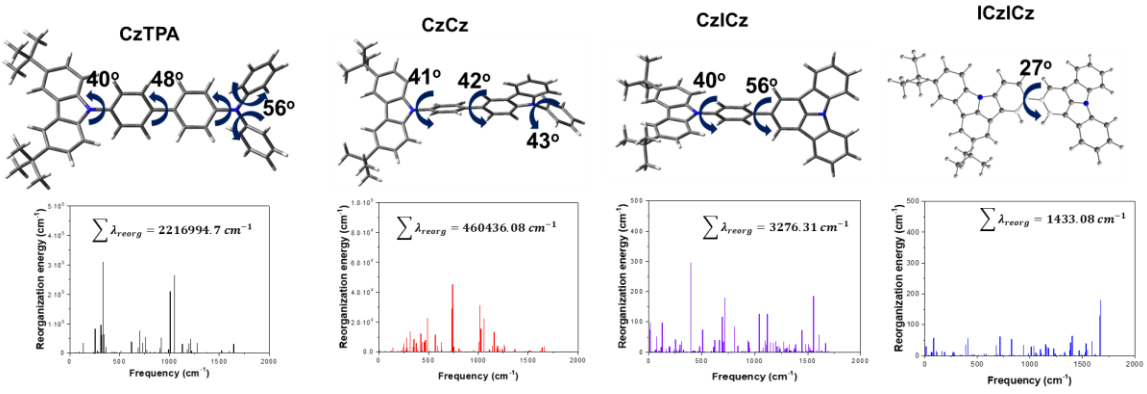



**Figure S2**. Optimized structure with dihedral angle and reorganisation energy of **CzTPA**, **CzCz**, **CzICz** and **ICzICz** computed by DFT methods

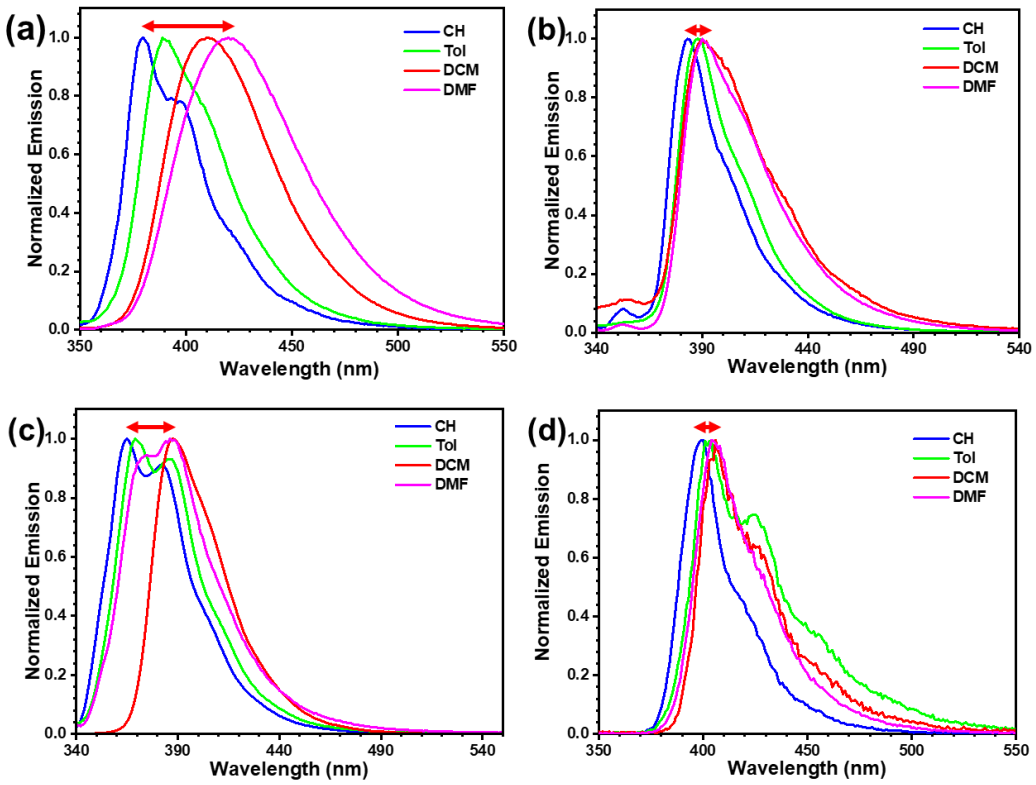



**Figure S3.** Solvatochromic analysis of compounds **CzTPA, CzCz, CzICz** and **ICzICz**

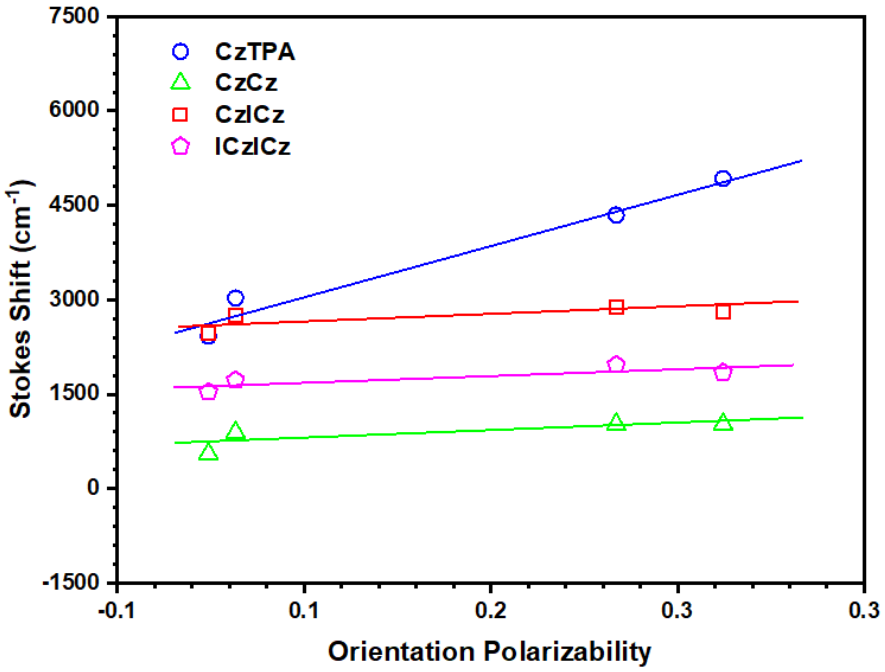



**Figure S4.** Lippert-Mataga plot of **CzTPA**, **CzCz**, **CzICz** and **ICzICz**

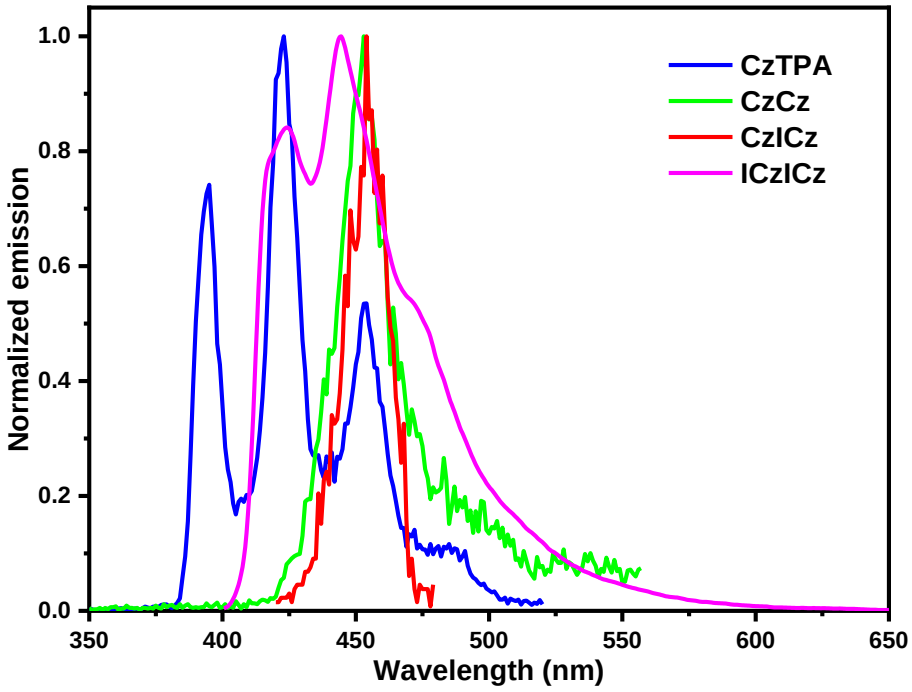



**Figure S5.** Phosphorescence spectra of **CzTPA**, **CzCz**, **CzICz** and **ICzICz** measured in frozen THF

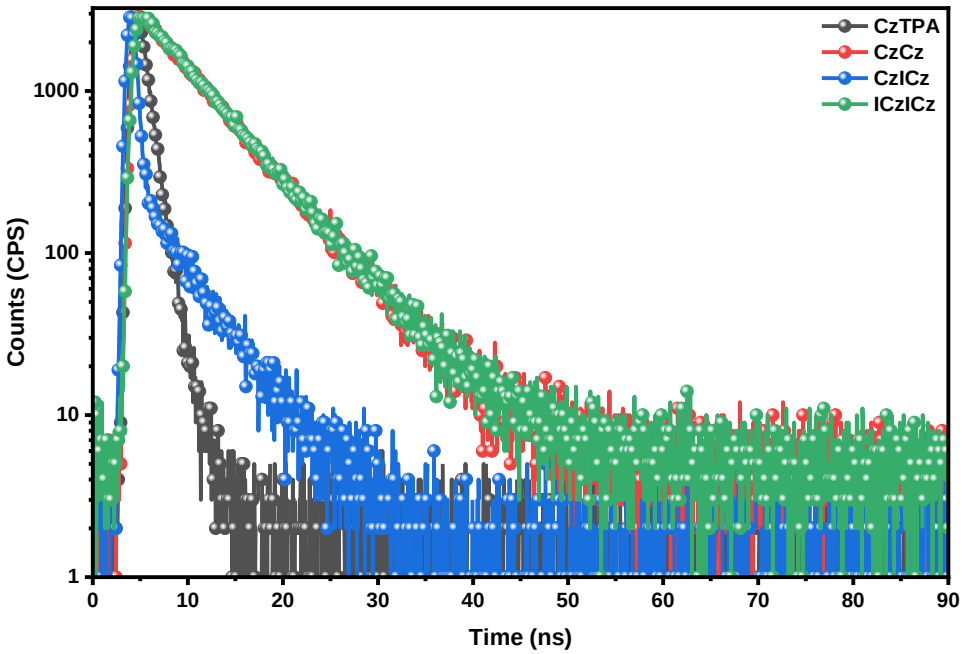



**Figure S6.** Time-resolved PL spectra of compounds collected in dilute DCM.

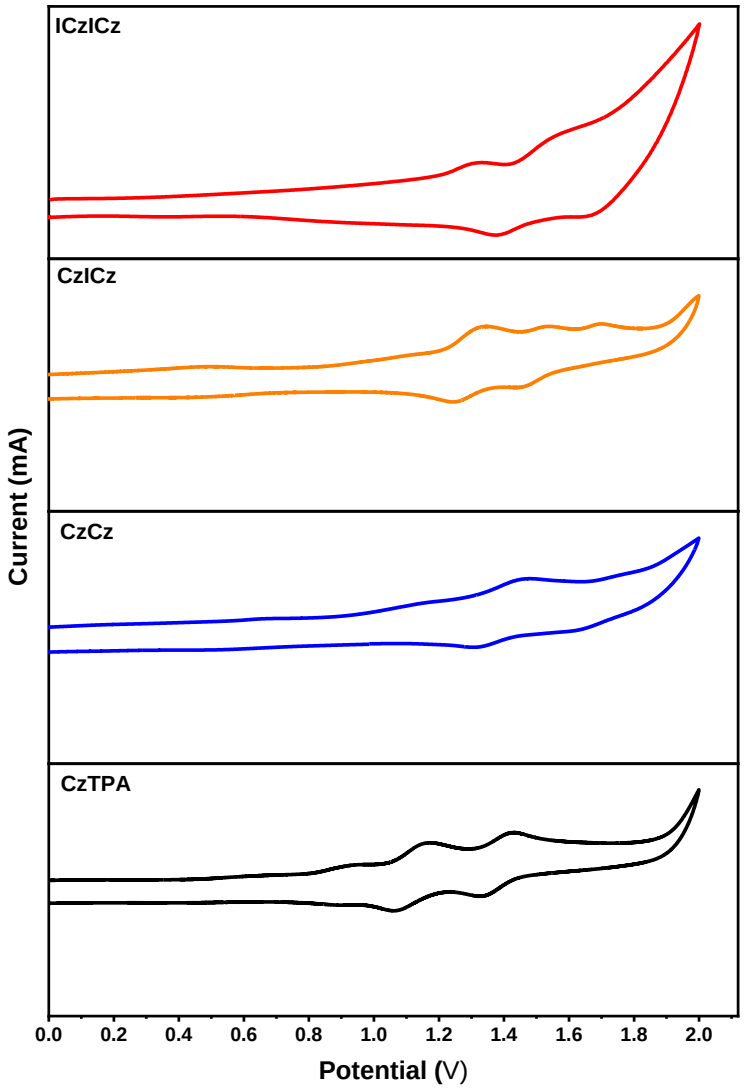



**Figure S7.** Cyclic Voltammograms of **CzTPA**, **CzCz**, **CzICz** and **ICzICz**

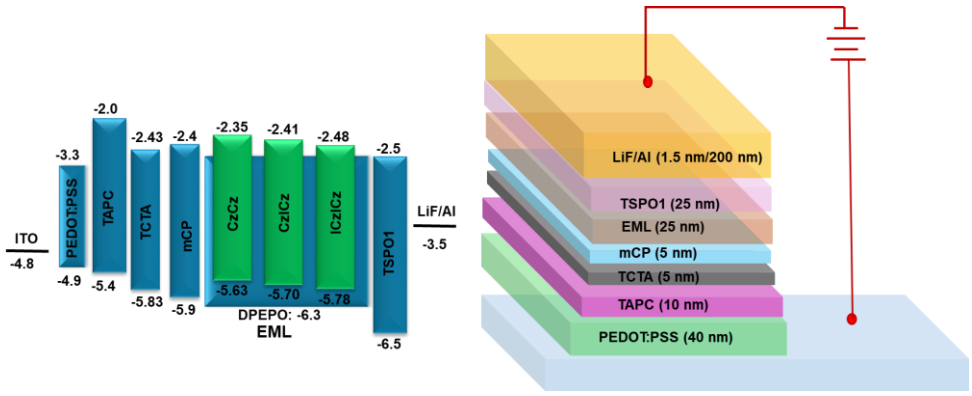



**Figure S8.** Fluorescent OLED device structure for **CzCz, CzICz** and **ICzICz** (all values in energy stack are in eV)

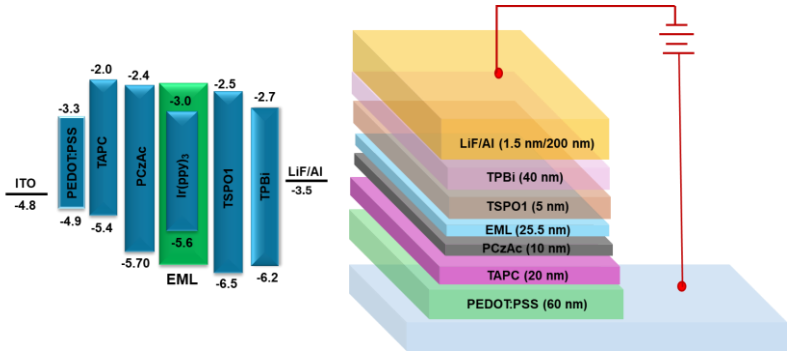



**Figure S9.** Phosphorescent OLED device structure for **CzCz, CzICz** and **ICzICz** (all values in energy stack are in eV)

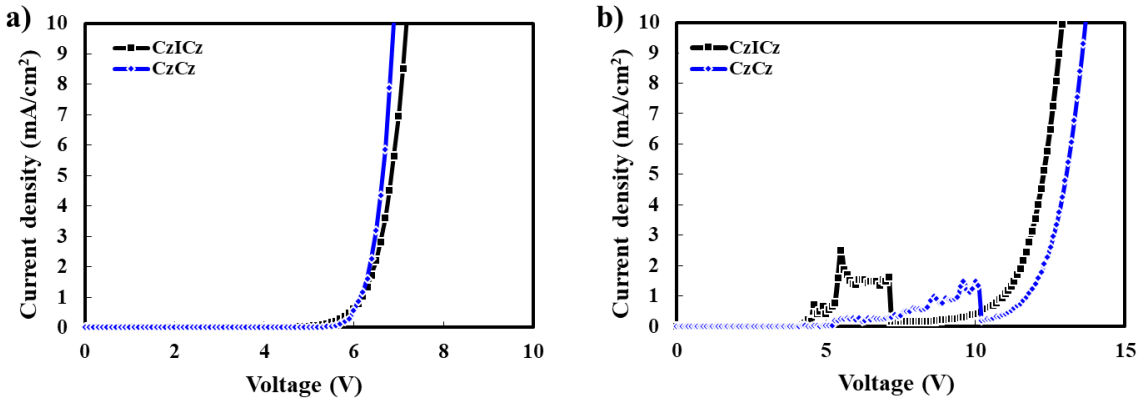



**Figure S10.** a) Hole only (HOD) and b) electron only (EOD) device studies of **CzICz** and **CzCz.**

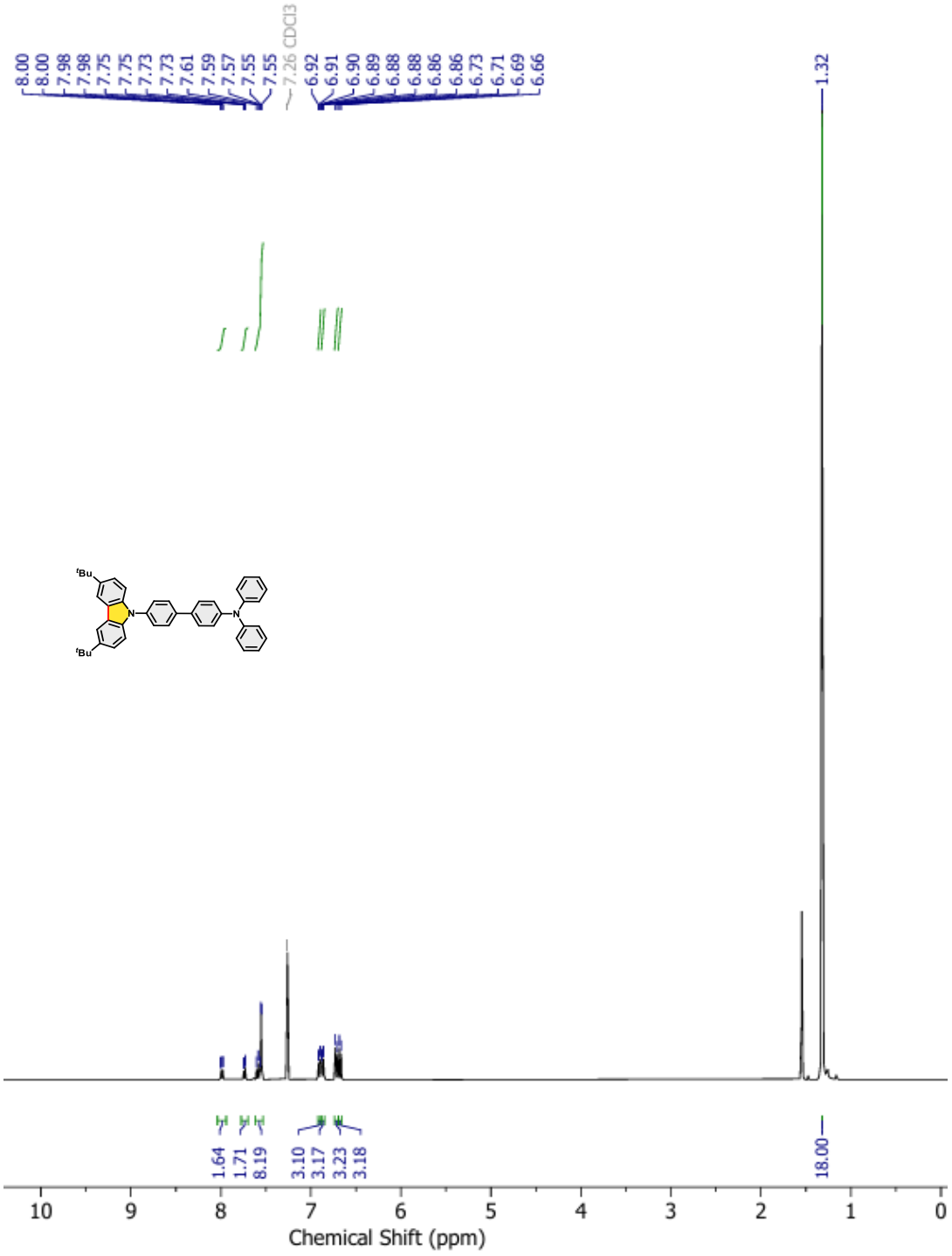



**Figure S11.** $^{1}$H NMR spectra of compound **CzTPA** recorded in $CDCl_3$

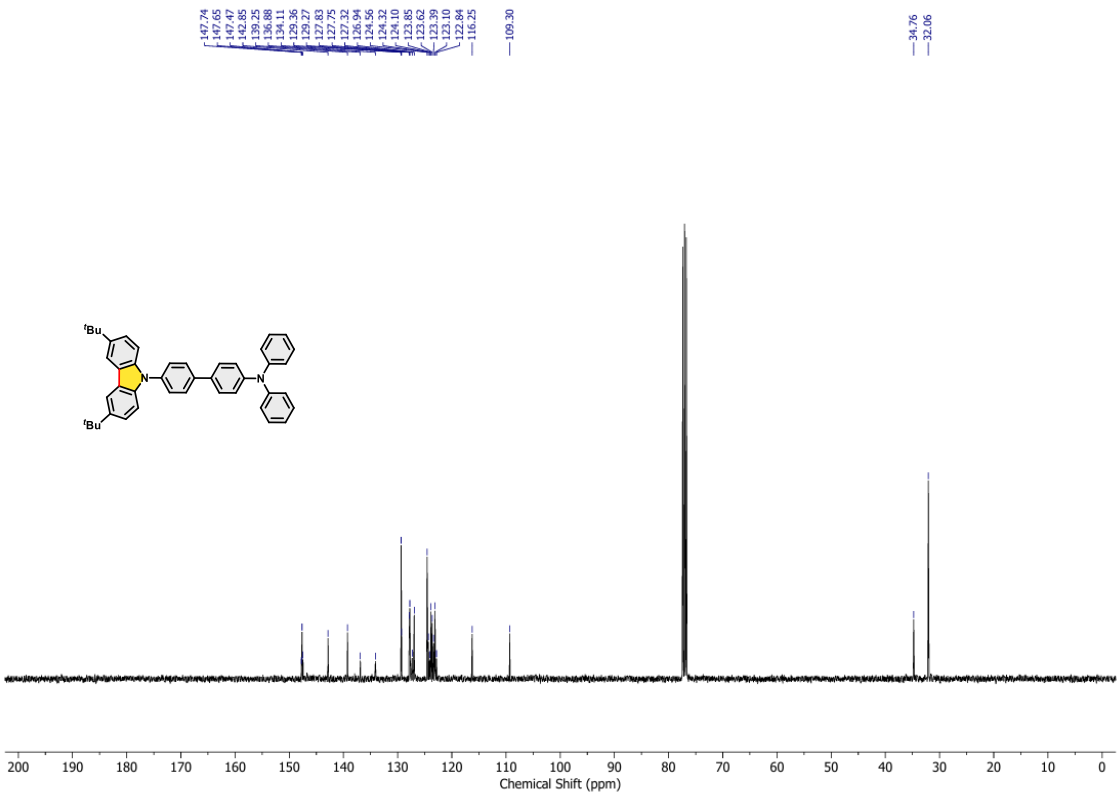



**Figure S12.** $^{13}C$ NMR spectra of compound **CzTPA** recorded in $CDCl_3$

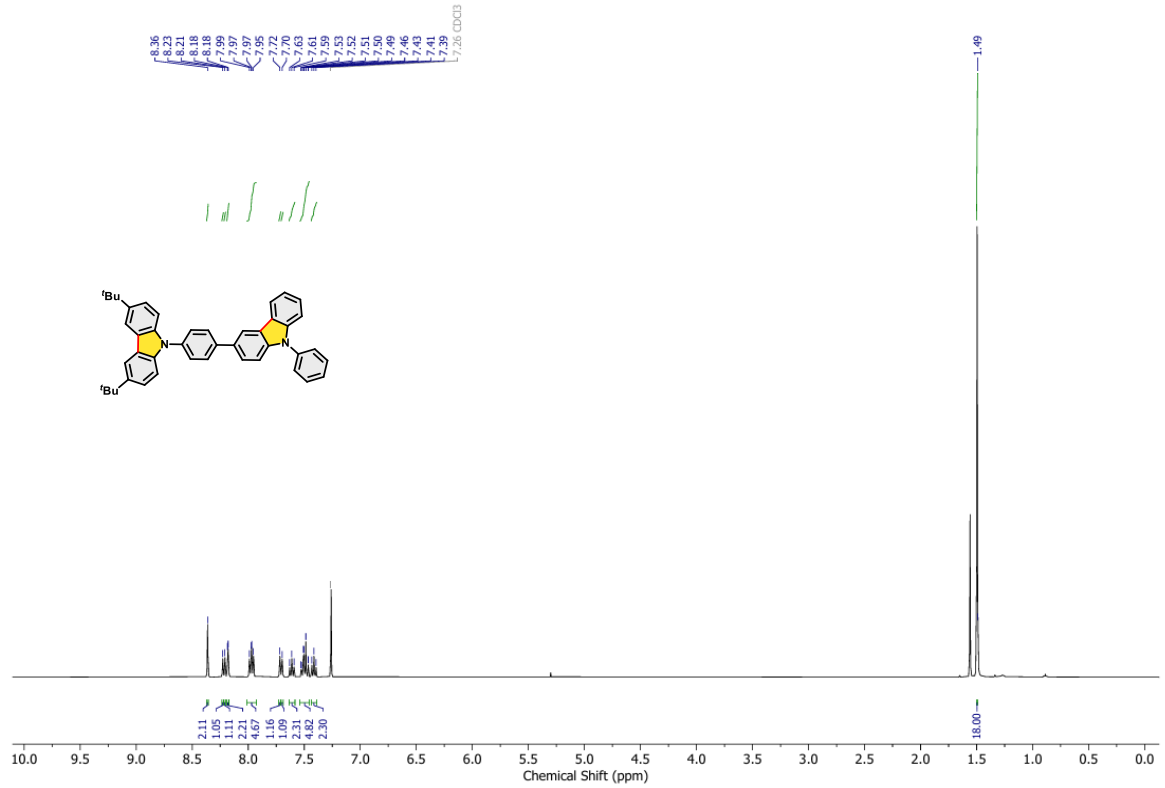



**Figure S13.** $^{1}H$ NMR spectra of compound **CzCz** recorded in $CDCl_3$

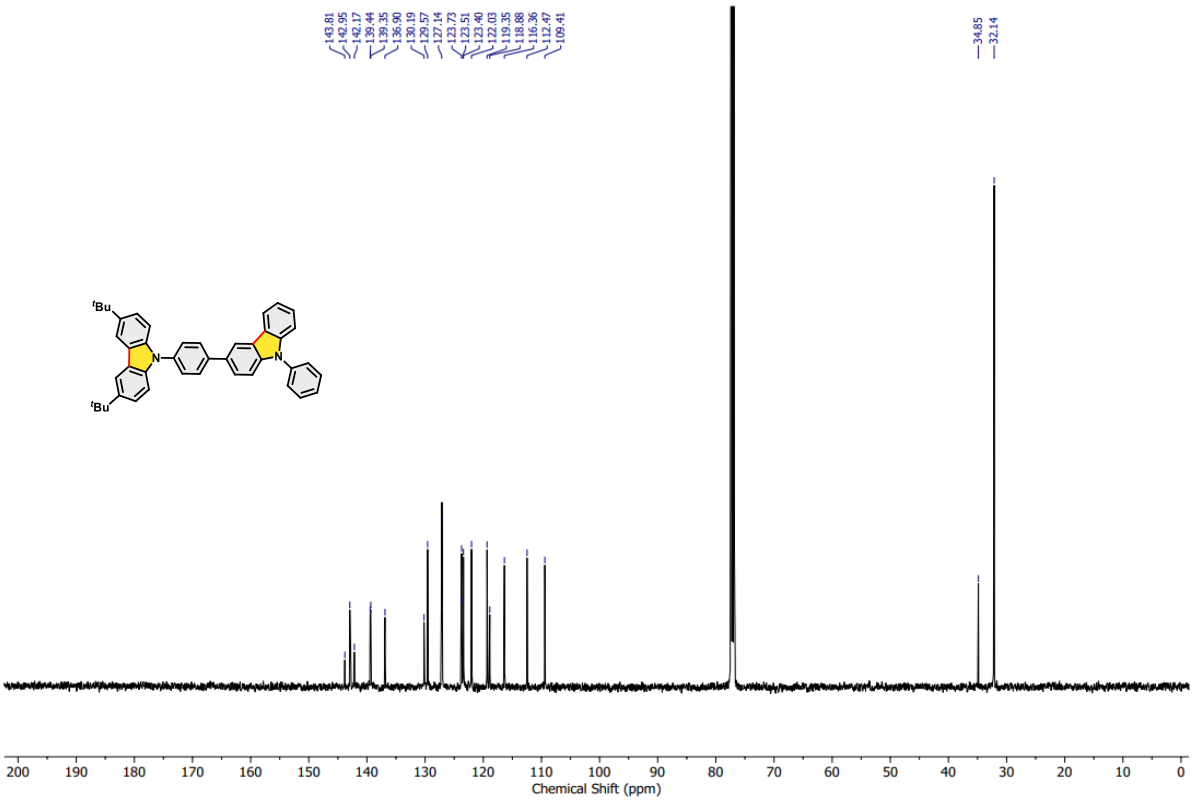



**Figure S14.** $^{13}$C NMR spectra of compound **CzCz** recorded in $CDCl_3$

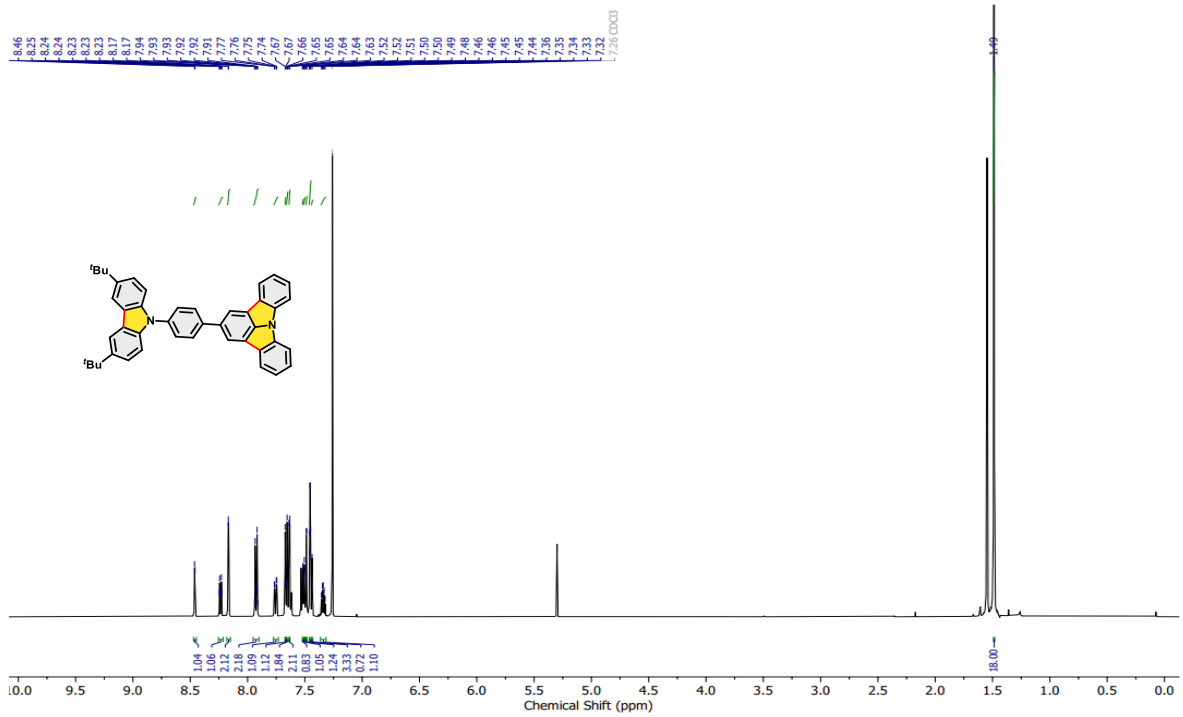



**Figure S15.** $^{1}$H NMR spectra of compound **CzICz** recorded in $CDCl_3$

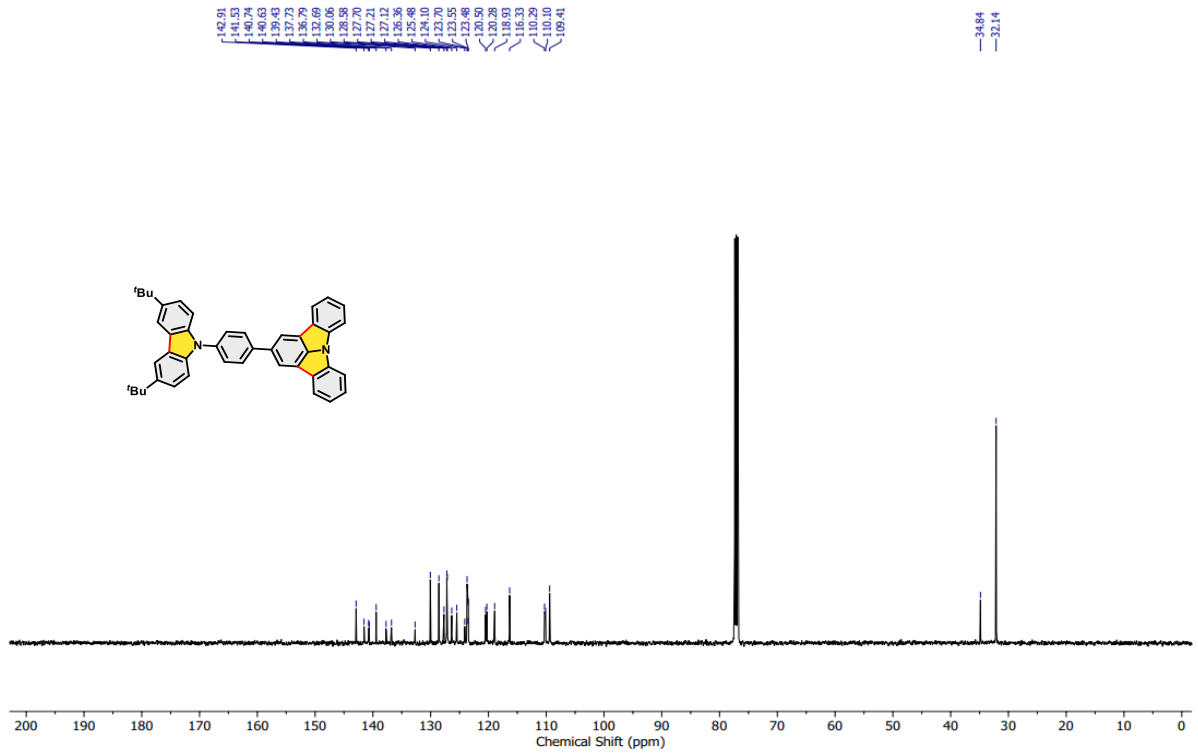



**Figure S16.** $^{13}C$ NMR spectra of compound **CzICz** recorded in $CDCl_3$

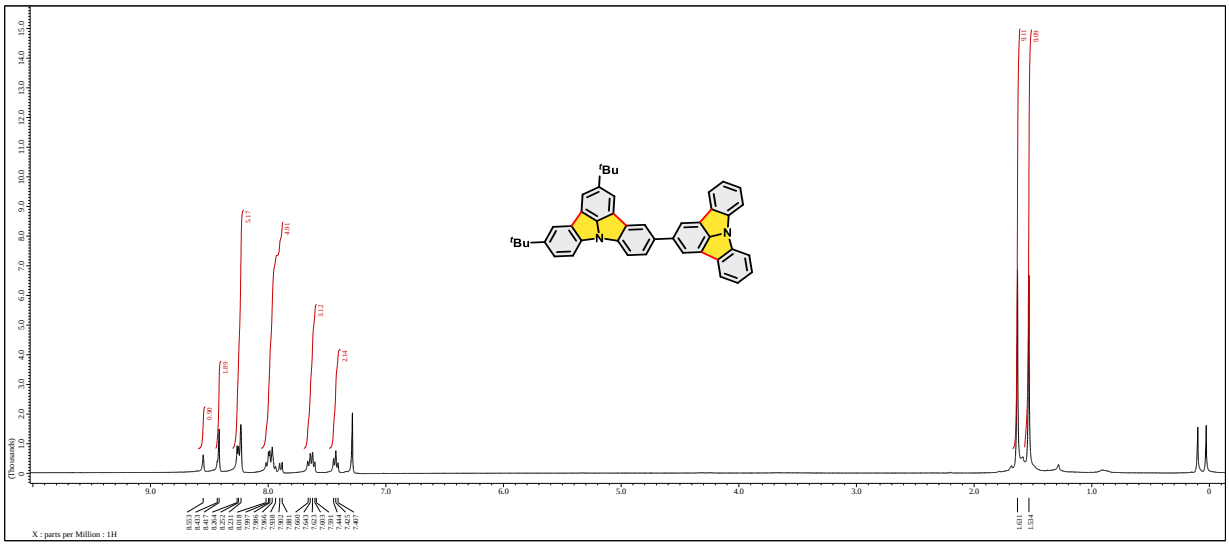



**Figure S17.** $^{1}H$ NMR spectra of compound **ICzICz** recorded in $CDCl_3$

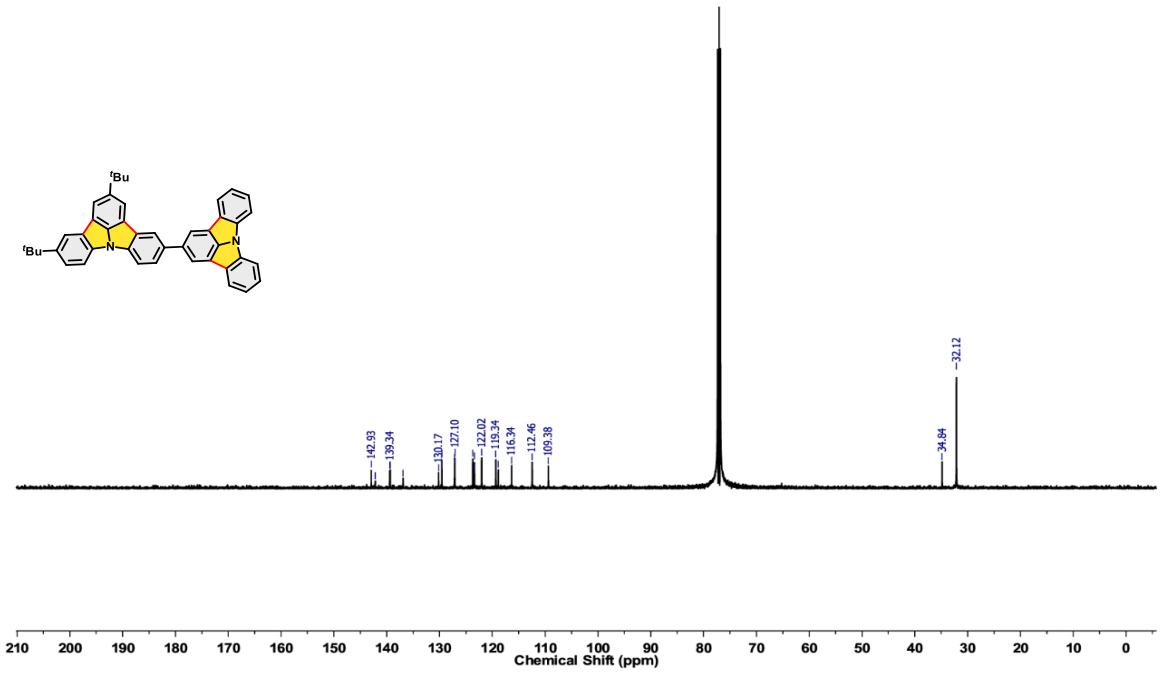
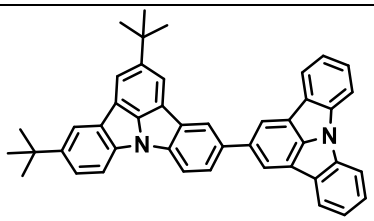
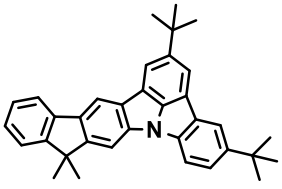
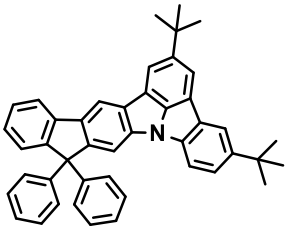
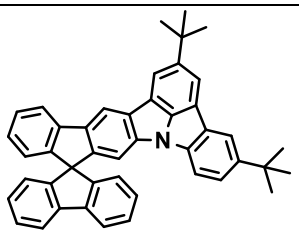
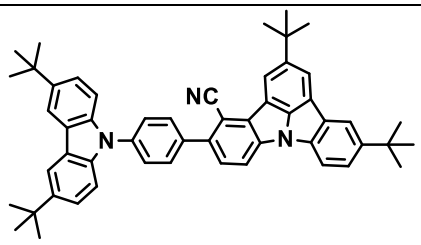
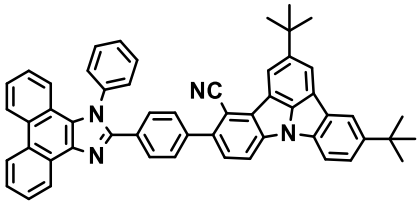
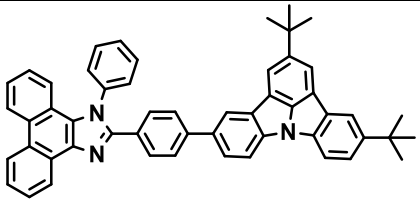
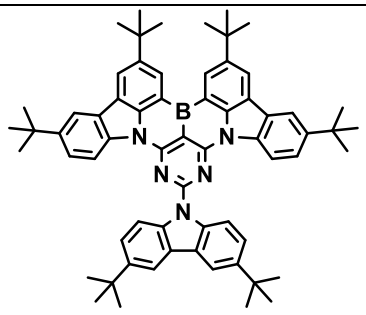
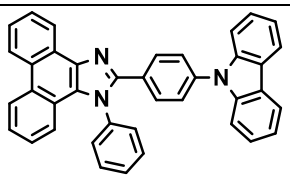
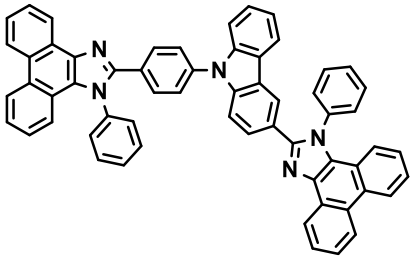
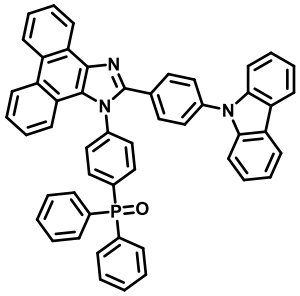
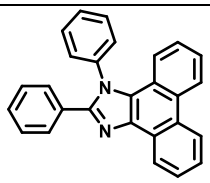
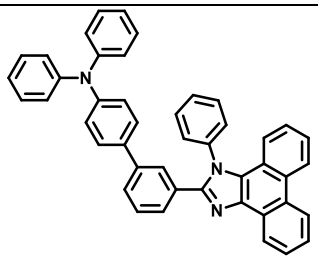
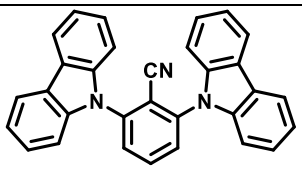
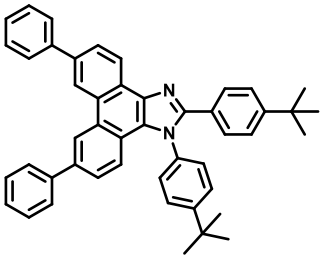
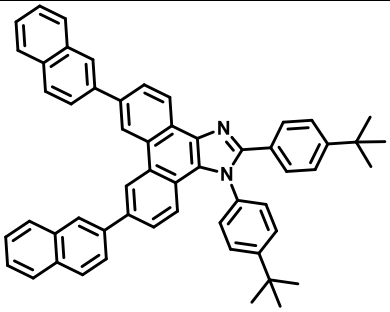



**Figure S18.** $^{13}C$ NMR spectra of compound **ICzICz** recorded in $CDCl_3$

**Table S1.** Comparison of CIEy and EQE of ICzICz with the reported UV emitters.

| SI. No. | Emitters | $\lambda_{PL}$ (nm) | $EQE_{max}$ (%) | CIEy | Ref. |
|---|---|---|---|---|---|
| 1. |  **ICzICz** | 398 | 4.2 | 0.029 | This work |
| 2. |  **tIDCz** | 399 | 2.92 | 0.051 | [2] |
| 3. |  **DPtIDCz** | 400 | 2.59 | 0.036 | [2] |

| | | | | | |
|---|---|---|---|---|---|
| 4. |  **SFtIDCz** | 399 | 2.41 | 0.033 | [2] |
| 5. |  **ICzICzCN** | 397 | 1.61 | 0.045 | [3] |
| 6. |  **ICzPICN** | 400 | 0.80 | 0.041 | [3] |
| 7. |  **ICzPI** | 403 | 3.07 | 0.046 | [3] |
| 8. |  **Pm-BN** | 409 | 2.5 | 0.045 | [4] |
| 9. |  **M1** | 399 | 1.94 | 0.05 | [5] |
| 10. |  | 407 | 3.02 | 0.056 | [5] |

| | M2 | | | | |
|---|---|---|---|---|---|
| 11. |  <br>**PhImPOCz** | 402 | 2.81 | 0.05 | [6] |
| 12. |  <br>**PPI** | 364 | 1.86 | 0.065 | [7] |
| 13. |  <br>**mTPA-PPI** | 367 | 3.33 | 0.049 | [7] |
| 14. |  <br>**DCzBN1** | 403 | 2.5 | 0.05 | [8] |
| 15. |  <br>**TPI-Bz** | 383 | 1.45 | 0.04 | [9] |
| 16. |  <br>**TPI-2Na** | 398 | 1.98 | 0.06 | [9] |

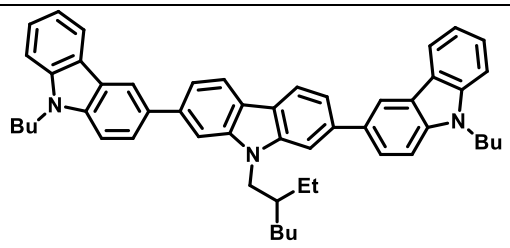
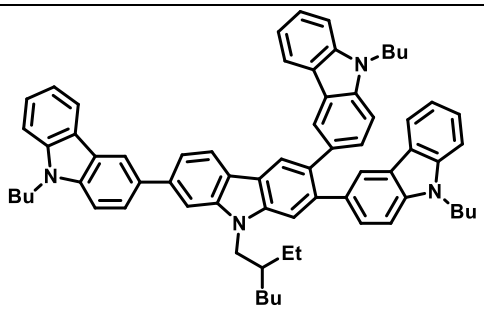
| | | | | | |
|---|---|---|---|---|---|
| 17. |  **1b** | 397 | 2.7 | 0.05 | [10] |
| 18. |  **2b** | 415 | 1.7 | 0.06 | [10] |

**Table S2.** Cartesian coordinates of the compound **CzTPA**

| | | | |
|---|---|---|---|
| C | -5.93626831 | -3.00549980 | 0.55024562 |
| C | -4.57304398 | -3.36596947 | 0.62427918 |
| C | -3.53569204 | -2.44605282 | 0.45162226 |
| C | -3.87235843 | -1.11768530 | 0.19196918 |
| C | -5.22972796 | -0.71502772 | 0.12335808 |
| C | -6.24391545 | -1.66031472 | 0.30048555 |
| H | -4.29930987 | -4.39505687 | 0.82452725 |
| H | -2.50150403 | -2.76521376 | 0.52505528 |
| H | -7.27946887 | -1.33687769 | 0.24531975 |
| C | -3.87235695 | 1.11768243 | -0.19198418 |
| C | -3.53569572 | 2.44605713 | -0.45161111 |

| | | | |
|---|---|---|---|
| C | -4.57305145 | 3.36597127 | -0.62425501 |
| C | -5.93627387 | 3.00549475 | -0.55022709 |
| C | -6.24391609 | 1.66031524 | -0.30043809 |
| C | -5.22972634 | 0.71502995 | -0.12330494 |
| H | -2.50151101 | 2.76523199 | -0.52499983 |
| H | -4.29932495 | 4.39506805 | -0.82446620 |
| H | -7.27947045 | 1.33689026 | -0.24521951 |
| N | -3.05074404 | -0.00000542 | -0.00000668 |
| C | -1.63054787 | -0.00000789 | 0.00000593 |
| C | -0.92083676 | -0.81772670 | -0.88894730 |
| C | -0.92085737 | 0.81771962 | 0.88897014 |
| C | 0.47266604 | -0.81948133 | -0.88126905 |
| H | -1.46464251 | -1.43454328 | -1.59742951 |
| C | 0.47264692 | 0.81950954 | 0.88129026 |
| H | -1.46467941 | 1.43449336 | 1.59747675 |
| C | 1.20201655 | 0.00002699 | 0.00000693 |
| H | 1.00211866 | -1.43982145 | -1.59811466 |
| H | 1.00208555 | 1.43986057 | 1.59813736 |
| C | 2.68488442 | 0.00005811 | 0.00000548 |
| C | 3.41740952 | 1.18032230 | 0.22241131 |

| | | | |
|---|---|---|---|
| C | 3.41744602 | -1.18017307 | -0.22240265 |
| C | 4.80936767 | 1.18717507 | 0.21625662 |
| H | 2.89119500 | 2.11991346 | 0.36360179 |
| C | 4.80941230 | -1.18697389 | -0.21625586 |
| H | 2.89126553 | -2.11978317 | -0.36359159 |
| C | 5.53017488 | 0.00011040 | -0.00000209 |
| H | 5.34499772 | 2.11819506 | 0.36964869 |
| H | 5.34507371 | -2.11797562 | -0.36965410 |
| N | 6.94822703 | 0.00012745 | -0.00005306 |
| C | 7.66278873 | -0.79155581 | -0.94275870 |
| C | 8.78490988 | -1.53571011 | -0.54206773 |
| C | 7.25900971 | -0.83795919 | -2.28762387 |
| C | 9.48962316 | -2.30220888 | -1.47085906 |
| H | 9.10113874 | -1.50815086 | 0.49563537 |
| C | 7.95925975 | -1.62040475 | -3.20635719 |
| H | 6.39746422 | -0.26040369 | -2.60664267 |
| C | 9.08039811 | -2.35416952 | -2.80675545 |
| H | 10.35505857 | -2.87151516 | -1.14360047 |
| H | 7.63352676 | -1.64400696 | -4.24248496 |
| H | 9.62714304 | -2.95666967 | -3.52561603 |

| | | | |
|---|---|---|---|
| C | 7.66292086 | 0.79163275 | 0.94268707 |
| C | 8.78528215 | 1.53547179 | 0.54205511 |
| C | 7.25909110 | 0.83816473 | 2.28753332 |
| C | 9.49013699 | 2.30180069 | 1.47087155 |
| H | 9.10158203 | 1.50779904 | -0.49562160 |
| C | 7.95950079 | 1.62044183 | 3.20629337 |
| H | 6.39739924 | 0.26081674 | 2.60652762 |
| C | 9.08084664 | 2.35390628 | 2.80674762 |
| H | 10.35574555 | 2.87086667 | 1.14365437 |
| H | 7.63371541 | 1.64413474 | 4.24240336 |
| H | 9.62770614 | 2.95628500 | 3.52562271 |
| C | -7.07612902 | 4.02804780 | -0.73674085 |
| C | -7.94941044 | 4.07059450 | 0.54120600 |
| C | -6.55239716 | 5.45365241 | -1.00145395 |
| C | -7.95601134 | 3.61221699 | -1.94115428 |
| H | -8.39331760 | 3.09510836 | 0.76261536 |
| H | -7.35470332 | 4.37136739 | 1.41058573 |
| H | -8.76781295 | 4.79059073 | 0.42160386 |
| H | -5.95239430 | 5.50558402 | -1.91643740 |
| H | -7.39892735 | 6.13789939 | -1.12378394 |

| | | | |
|---|---|---|---|
| H | -5.94477748 | 5.82680329 | -0.16990354 |
| H | -8.77304731 | 4.32957836 | -2.08355924 |
| H | -7.36550266 | 3.57997937 | -2.86319213 |
| H | -8.40230927 | 2.62349412 | -1.79651901 |
| C | -7.07612282 | -4.02805453 | 0.73675647 |
| C | -7.95614771 | -3.61209599 | 1.94102120 |
| C | -7.94926259 | -4.07076777 | -0.54128123 |
| C | -6.55239742 | -5.45361923 | 1.00169707 |
| H | -7.36574995 | -3.57976237 | 2.86312685 |
| H | -8.40242374 | -2.62338555 | 1.79622733 |
| H | -8.77320416 | -4.32943818 | 2.08340581 |
| H | -7.35444947 | -4.37161530 | -1.41056232 |
| H | -8.76765261 | -4.79077966 | -0.42168810 |
| H | -8.39317933 | -3.09532167 | -0.76284424 |
| H | -7.39893000 | -6.13786420 | 1.12402348 |
| H | -5.94468985 | -5.82686282 | 0.17025137 |
| H | -5.95248526 | -5.50543093 | 1.91674540 |

**Table S3.** Cartesian Coordinates of the compound **CzCz**

| | | | |
|---|---|---|---|
| C | 5.80958428 | 3.03246519 | 0.15997395 |
| C | 4.44088800 | 3.39889792 | 0.18486429 |

| | | | |
|---|---|---|---|
| C | 3.40570092 | 2.46794452 | 0.17115498 |
| C | 3.74596226 | 1.11229265 | 0.13446991 |
| C | 5.10105747 | 0.70655090 | 0.09567599 |
| C | 6.12022286 | 1.67042564 | 0.11133070 |
| H | 4.17267090 | 4.45057260 | 0.21419510 |
| H | 2.37058986 | 2.79266279 | 0.18338711 |
| H | 7.15197133 | 1.33895699 | 0.08138683 |
| C | 3.74696900 | -1.15000252 | 0.03064904 |
| C | 3.40885648 | -2.50642516 | 0.00393551 |
| C | 4.44530608 | -3.43504130 | -0.03974375 |
| C | 5.81332043 | -3.06557167 | -0.05469318 |
| C | 6.12217955 | -1.70283534 | -0.01507470 |
| C | 5.10171536 | -0.74126059 | 0.03017263 |
| H | 2.37459972 | -2.83357630 | 0.02164798 |
| H | 4.17866860 | -4.48730327 | -0.06127070 |
| H | 7.15360332 | -1.36901098 | -0.01520009 |
| N | 2.92495491 | -0.01973627 | 0.09429518 |
| C | 1.50354327 | -0.02147559 | 0.11632972 |
| C | 0.81038148 | 0.56348160 | 1.18344704 |
| C | 0.77898140 | -0.60930478 | -0.92812014 |

| | | | |
|---|---|---|---|
| C | -0.58358853 | 0.56849992 | 1.19616813 |
| H | 1.36699580 | 1.01552662 | 1.99842355 |
| C | -0.61459809 | -0.62005191 | -0.89611258 |
| H | 1.31099909 | -1.06018399 | -1.75998143 |
| C | -1.32770889 | -0.02662822 | 0.16130621 |
| H | -1.10218710 | 1.05252102 | 2.01830783 |
| H | -1.15765531 | -1.10783662 | -1.70001604 |
| C | -2.81339095 | -0.02799435 | 0.18358892 |
| C | -3.54882076 | 0.17681873 | -0.99193291 |
| C | -3.51237265 | -0.24224501 | 1.39628441 |
| C | -4.94663948 | 0.17412620 | -0.95370465 |
| H | -3.03224550 | 0.36052722 | -1.92952548 |
| C | -4.90310065 | -0.24988896 | 1.46268714 |
| H | -2.94665690 | -0.43512473 | 2.30268954 |
| C | -5.61615587 | -0.03208765 | 0.27977318 |
| H | -5.41068354 | -0.43442928 | 2.40338974 |
| N | -6.99540885 | -0.00266150 | 0.06192011 |
| C | -7.22229963 | 0.22412127 | -1.30030949 |
| C | -8.43342934 | 0.35988576 | -1.98671300 |
| C | -5.97280599 | 0.34168014 | -1.96330571 |

| | | | |
|---|---|---|---|
| C | -8.37640843 | 0.60288519 | -3.35904719 |
| H | -9.38539217 | 0.28444902 | -1.47229556 |
| C | -5.94367309 | 0.58558534 | -3.34264064 |
| C | -7.14654023 | 0.71207959 | -4.03475765 |
| H | -9.30281036 | 0.71219752 | -3.91527887 |
| H | -4.99591035 | 0.67870116 | -3.86535969 |
| H | -7.13754104 | 0.90067321 | -5.10387763 |
| C | -7.99933239 | -0.17351296 | 1.05734093 |
| C | -8.90679585 | -1.23636186 | 0.96225922 |
| C | -8.07960180 | 0.72071321 | 2.13253469 |
| C | -9.89479634 | -1.39625659 | 1.93608559 |
| H | -8.82812228 | -1.93233292 | 0.13307406 |
| C | -9.05914620 | 0.54439623 | 3.11207396 |
| H | -7.38154303 | 1.54990317 | 2.19003960 |
| C | -9.97119065 | -0.51043486 | 3.01475916 |
| H | -10.59707366 | -2.22087205 | 1.85704672 |
| H | -9.11611557 | 1.23935059 | 3.94467734 |
| H | -10.73616319 | -0.64125024 | 3.77416649 |
| C | 6.89310523 | -4.16431359 | -0.10927221 |
| C | 6.76027545 | -5.08798789 | 1.12655998 |

| | | | |
|---|---|---|---|
| C | 6.71372616 | -5.00654798 | -1.39635973 |
| C | 8.32072856 | -3.58326226 | -0.11688239 |
| H | 6.89090925 | -4.51976156 | 2.05389050 |
| H | 5.78080974 | -5.57427578 | 1.16865206 |
| H | 7.52256475 | -5.87573604 | 1.09822144 |
| H | 6.81169195 | -4.37972262 | -2.28935866 |
| H | 7.47496679 | -5.79423682 | -1.44673500 |
| H | 5.73229498 | -5.48931589 | -1.43369349 |
| H | 9.04936076 | -4.40007556 | -0.15796877 |
| H | 8.49542605 | -2.94144364 | -0.98722480 |
| H | 8.52912221 | -3.00099701 | 0.78726926 |
| C | 6.88807985 | 4.13357640 | 0.18276073 |
| C | 6.74427567 | 4.97610203 | 1.47413456 |
| C | 8.31660150 | 3.55565118 | 0.14928121 |
| C | 6.71745326 | 5.05630685 | -1.04913580 |
| H | 5.76333504 | 5.45686912 | 1.53965386 |
| H | 6.86938735 | 4.34990836 | 2.36418771 |
| H | 7.50501638 | 5.76538226 | 1.50208804 |
| H | 8.49999365 | 2.97332533 | -0.76022632 |
| H | 9.04432907 | 4.37406781 | 0.16881633 |

| | | | |
|---|---|---|---|
| H | 8.51785634 | 2.91469988 | 1.01451770 |
| H | 7.47842136 | 5.84582155 | -1.04325826 |
| H | 6.82253458 | 4.48788427 | -1.97958658 |
| H | 5.73604706 | 5.54029672 | -1.06315464 |

**Table S4.** Cartesian coordinates of the compound **CzICz**

| | | | |
|---|---|---|---|
| C | -5.57885771 | -3.02885824 | 0.36347487 |
| C | -4.21053427 | -3.39552947 | 0.39931025 |
| C | -3.17423602 | -2.47182658 | 0.29239606 |
| C | -3.51286809 | -1.12311375 | 0.14701161 |
| C | -4.86773872 | -0.71860009 | 0.09356982 |
| C | -5.88808217 | -1.67489670 | 0.20484340 |
| H | -3.94333399 | -4.44168190 | 0.51320130 |
| H | -2.13975830 | -2.79776248 | 0.31665441 |
| H | -6.91961225 | -1.34422243 | 0.16175073 |
| C | -3.51276892 | 1.12285426 | -0.14787509 |
| C | -3.17393244 | 2.47152644 | -0.29315479 |
| C | -4.21010662 | 3.39541629 | -0.39958500 |
| C | -5.57848316 | 3.02894153 | -0.36338149 |
| C | -5.88789325 | 1.67502155 | -0.20482091 |
| C | -4.86767192 | 0.71854034 | -0.09397013 |

| | | | |
|---|---|---|---|
| H | -2.13939151 | 2.79725645 | -0.31764022 |
| H | -3.94280519 | 4.44155541 | -0.51336675 |
| H | -6.91947794 | 1.34454911 | -0.16143805 |
| N | -2.69099537 | -0.00020337 | -0.00068104 |
| C | -1.26989645 | -0.00018462 | -0.00050984 |
| C | -0.56096264 | -0.50658308 | 1.09609206 |
| C | -0.56085706 | 0.50629431 | -1.09701934 |
| C | 0.83315026 | -0.51499636 | 1.08712188 |
| H | -1.10512067 | -0.89550621 | 1.95098785 |
| C | 0.83324663 | 0.51486071 | -1.08786917 |
| H | -1.10497503 | 0.89514982 | -1.95197909 |
| C | 1.56122049 | -0.00003192 | -0.00032088 |
| H | 1.36488537 | -0.93879006 | 1.93385905 |
| H | 1.36505878 | 0.93870275 | -1.93453404 |
| C | 3.05080278 | 0.00004894 | -0.00021483 |
| C | 3.73615083 | -0.38144058 | -1.18696254 |
| C | 3.73593733 | 0.38156031 | 1.18664899 |
| C | 5.13719447 | -0.38397815 | -1.20005008 |
| H | 3.15602525 | -0.68703487 | -2.05202606 |
| C | 5.13697944 | 0.38425098 | 1.19994033 |

| | | | |
|---|---|---|---|
| H | 3.15565138 | 0.68700288 | 2.05165832 |
| C | 5.71272537 | 0.00024525 | -0.00003778 |
| N | 7.07767194 | 0.00024173 | 0.00008565 |
| C | 7.48450399 | -0.41348160 | -1.27995028 |
| C | 8.75976634 | -0.58504467 | -1.81109870 |
| C | 6.29768473 | -0.66480472 | -2.05809856 |
| C | 8.86104382 | -1.01500685 | -3.13833597 |
| H | 9.64836247 | -0.39354002 | -1.21934300 |
| C | 6.43848853 | -1.09254793 | -3.37996240 |
| C | 7.71894666 | -1.26579946 | -3.91340405 |
| H | 9.84546147 | -1.15640125 | -3.57420803 |
| H | 5.56016870 | -1.28928469 | -3.98782868 |
| H | 7.83192182 | -1.59885823 | -4.94044060 |
| C | 7.48427422 | 0.41357802 | 1.28031934 |
| C | 8.75944137 | 0.58490940 | 1.81177096 |
| C | 6.29731520 | 0.66487617 | 2.05826293 |
| C | 8.86048131 | 1.01458696 | 3.13911847 |
| H | 9.64814339 | 0.39343186 | 1.22016542 |
| C | 6.43788262 | 1.09236410 | 3.38023451 |
| C | 7.71824513 | 1.26536300 | 3.91398724 |

| | | | |
|---|---|---|---|
| H | 9.84482074 | 1.15577012 | 3.57523532 |
| H | 5.55945426 | 1.28908865 | 3.98794784 |
| H | 7.83103608 | 1.59821133 | 4.94111234 |
| C | -6.65787282 | 4.12171716 | -0.49393114 |
| C | -6.50519794 | 5.14555724 | 0.65779421 |
| C | -6.49701458 | 4.85225572 | -1.84983250 |
| C | -8.08599273 | 3.54530717 | -0.43119964 |
| H | -6.62206086 | 4.65746969 | 1.63144729 |
| H | -5.52483342 | 5.63163769 | 0.64392962 |
| H | -7.26716687 | 5.92975853 | 0.57504969 |
| H | -6.60980046 | 4.15293359 | -2.68541433 |
| H | -7.25767200 | 5.63511042 | -1.95460149 |
| H | -5.51550493 | 5.32733040 | -1.94249898 |
| H | -8.81433922 | 4.35744665 | -0.52963109 |
| H | -8.27460737 | 2.83323393 | -1.24195767 |
| H | -8.28118351 | 3.04137288 | 0.52163605 |
| C | -6.65841380 | -4.12142426 | 0.49441457 |
| C | -6.49718736 | -4.85207912 | 1.85020277 |
| C | -8.08646422 | -3.54476093 | 0.43224602 |
| C | -6.50635287 | -5.14525549 | -0.65739879 |

| | | | |
|---|---|---|---|
| H | -5.51576412 | -5.32742284 | 1.94243050 |
| H | -6.60946056 | -4.15279909 | 2.68588536 |
| H | -7.25798935 | -5.63476058 | 1.95522447 |
| H | -8.28196881 | -3.04086406 | -0.52054056 |
| H | -8.81490359 | -4.35677363 | 0.53103902 |
| H | -8.27460695 | -2.83260170 | 1.24303577 |
| H | -7.26842922 | -5.92932857 | -0.57440567 |
| H | -6.62346953 | -4.65712907 | -1.63100129 |
| H | -5.52606487 | -5.63150677 | -0.64388534 |

**Table S5.** Cartesian coordinates of the compound **ICzICz**

| | | | |
|---|---|---|---|
| C | 5.17594437 | -0.40975349 | 0.07727529 |
| C | 6.51812129 | -0.77170488 | 0.15625467 |
| C | 6.89840452 | -2.09136987 | 0.45681888 |
| C | 5.88270636 | -3.03948540 | 0.67596119 |
| C | 4.52240913 | -2.72085735 | 0.60672459 |
| C | 4.17005247 | -1.41275667 | 0.30906262 |
| N | 2.91210745 | -0.80059759 | 0.17353449 |
| C | 3.14771200 | 0.51156526 | -0.12636134 |
| C | 1.51815745 | -0.95963974 | 0.21484363 |
| C | 0.73726703 | -2.08163949 | 0.46818581 |

| | | | |
|---|---|---|---|
| C | -0.64986498 | -1.93634665 | 0.44059187 |
| C | -1.27464092 | -0.70291734 | 0.16223543 |
| C | -0.47065109 | 0.42086166 | -0.09418404 |
| C | 0.91827639 | 0.31768217 | -0.07111439 |
| C | 2.00882604 | 1.27847797 | -0.29723215 |
| C | 2.26836291 | 2.61894593 | -0.60393150 |
| C | 3.60919305 | 3.08054668 | -0.71369465 |
| C | 4.70794014 | 2.20612954 | -0.51773723 |
| C | 4.48273248 | 0.85576932 | -0.20905956 |
| C | 3.82990091 | 4.57274852 | -1.05540409 |
| C | 5.32166296 | 4.94943155 | -1.14431379 |
| C | 3.18549518 | 5.45776095 | 0.03865203 |
| C | 3.18070438 | 4.89454295 | -2.42305272 |
| C | 8.39586913 | -2.44912046 | 0.53515082 |
| C | 9.06869737 | -2.15944791 | -0.82784106 |
| C | 8.62963890 | -3.93342159 | 0.87538433 |
| C | 9.07491303 | -1.59481510 | 1.63214211 |
| C | -2.76000419 | -0.59434111 | 0.14204881 |
| C | -3.51600480 | -1.62328663 | -0.48271366 |
| C | -4.91304434 | -1.53456042 | -0.50587340 |

| | | | |
|---|---|---|---|
| C | -5.41445472 | -0.39798619 | 0.10554810 |
| C | -4.76828013 | 0.65351430 | 0.73309632 |
| C | -3.37330205 | 0.53558937 | 0.74843204 |
| N | -6.77598354 | -0.29771906 | 0.08762019 |
| C | -7.10356114 | 0.89893308 | 0.74776718 |
| C | -7.25792670 | -1.43538210 | -0.58204774 |
| C | -6.12128810 | -2.23074799 | -0.96980258 |
| C | -6.34129867 | -3.42460709 | -1.65780334 |
| C | -7.64850586 | -3.81723170 | -1.95198690 |
| C | -8.74003353 | -3.02839738 | -1.56483900 |
| C | -8.56001425 | -1.82703903 | -0.87456150 |
| C | -8.34146971 | 1.47734738 | 1.00742233 |
| C | -8.36159332 | 2.69280154 | 1.69621444 |
| C | -7.17684129 | 3.31358446 | 2.11402174 |
| C | -5.93398390 | 2.73335800 | 1.85301680 |
| C | -5.87329220 | 1.51956491 | 1.16741322 |
| H | 7.27648372 | -0.01355866 | -0.01880962 |
| H | 6.14561363 | -4.06459473 | 0.90966264 |
| H | 3.77019360 | -3.48344459 | 0.78318508 |
| H | 1.18729359 | -3.04332591 | 0.69365623 |

| | | | |
|---|---|---|---|
| H | -1.27017717 | -2.79869638 | 0.66656915 |
| H | -0.93848293 | 1.37113056 | -0.33610375 |
| H | 1.45300236 | 3.31836392 | -0.76125344 |
| H | 5.71841646 | 2.58612468 | -0.60791608 |
| H | 5.41686359 | 6.01380675 | -1.38710399 |
| H | 5.84409526 | 4.78058917 | -0.19579568 |
| H | 5.84054380 | 4.38589679 | -1.92807920 |
| H | 3.33256536 | 6.52011073 | -0.19257667 |
| H | 2.10801945 | 5.28339074 | 0.12520241 |
| H | 3.63487700 | 5.25744622 | 1.01803066 |
| H | 3.32808695 | 5.95152973 | -2.67753968 |
| H | 3.62644317 | 4.28763098 | -3.21940562 |
| H | 2.10304696 | 4.70100808 | -2.42125611 |
| H | 10.13759668 | -2.40300985 | -0.78663291 |
| H | 8.61349206 | -2.75900602 | -1.62438924 |
| H | 8.97870861 | -1.10558686 | -1.11152633 |
| H | 9.70568856 | -4.13610610 | 0.91940024 |
| H | 8.20396787 | -4.20145052 | 1.84913255 |
| H | 8.19988104 | -4.59899233 | 0.11805563 |
| H | 10.14389283 | -1.83305476 | 1.69598993 |

| | | | |
|---|---|---|---|
| H | 8.98502508 | -0.52261157 | 1.42843486 |
| H | 8.62430162 | -1.78667535 | 2.61260457 |
| H | -2.98756395 | -2.44767221 | -0.95202267 |
| H | -2.74220379 | 1.27351855 | 1.23454754 |
| H | -5.50086952 | -4.04262642 | -1.96212456 |
| H | -7.82214447 | -4.74586257 | -2.48796426 |
| H | -9.74843571 | -3.35389766 | -1.80462195 |
| H | -9.41073511 | -1.22167182 | -0.57836074 |
| H | -9.26363336 | 1.00287595 | 0.68738878 |
| H | -9.31737866 | 3.16278226 | 1.91049565 |
| H | -7.22658199 | 4.25820227 | 2.64787328 |
| H | -5.02034954 | 3.22185402 | 2.18091271 |

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