Abstract: In this study, we developed two thermally activated delayed fluorescence (TADF) emitters, ICzCN and ICzCYP, to apply to organic light-emitting diodes (OLEDs). These emitters involve indolocarbazole (ICz) donor units and nicotinonitrile acceptor units with a twisted donor-acceptor-donor (D-A-D) structure for small singlet ($S_1$) and triplet ($T_1$) state energy gap ($\Delta E_{ST}$) to enable efficient exciton transfer from the $T_1$ to the $S_1$ state. Depending on the position of the cyano-substituent, ICzCN has a symmetric structure by introducing donor units at the 3,5-position of isonicotinonitrile, and ICzCYP has an asymmetric structure by introducing donor units at the 2,6-position of nicotinonitrile. These emitters have different properties, such as the maximum luminance ($L_{\text{max}}$) value. The $L_{\text{max}}$ of ICzCN reached over 10000 cd m$^{-2}$. The external quantum efficiency ($\eta_{\text{ext}}$) was 14.8% for ICzCN and 14.9% for ICzCYP, and both achieved a low turn-on voltage ($V_{\text{on}}$) of less than 3.4 eV.

Keywords: organic light-emitting diodes; thermally activated delayed fluorescence; nicotinocarbonitrile; indolocarbazole; symmetry

1. Introduction

Organic light-emitting diodes (OLEDs) have been researched actively as next-generation displays because of their advantages, such as flexibility, brightness, and light weight, since the first study in 1987 [1]. In recent decades, numerous studies about organic fluorescence and phosphorescence emitters in the visible region have been performed to enhance the internal quantum efficiency ($\eta_{\text{int}}$) [2–7]. However, despite the exceptional stability and reliability of fluorescence materials, a low exciton production efficiency ($\eta_{\text{ext}}$) of 25% of fluorescence materials in electrical excitation results in a low maximum $\eta_{\text{ext}}$ [8]. Phosphorescence emitters can achieve a maximum $\eta_{\text{int}}$ of nearly 100% with singlet ($S_1$) and triplet ($T_1$) exciton harvesting via intersystem crossing (ISC) using heavy atom effect from transition metals in phosphorescence emitters [9,10]. Nevertheless, the high density of $T_1$ excitons from a long radiative decay time causes a strong $T_1$ exciton annihilation process and a significant efficiency decrease under high current density [11].

Recently, thermally activated delayed fluorescence (TADF) materials have been researched as alternatives to fluorescence and phosphorescence materials in OLEDs because of their high $\eta_{\text{ST}}$ through reverse ISC (RISC) from the $T_1$ to the $S_1$ state, resulting in a maximum $\eta_{\text{int}}$ of 100% [12–16]. A small $S_1$ and $T_1$ state energy gap ($\Delta E_{ST}$) attained by minimizing the overlap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) can lead to efficient RISC. Accordingly, various studies have concentrated on molecular designs using twisted molecular frameworks between the donor and acceptor units to obtain a small $\Delta E_{ST}$ with spatially separated and promoted
intramolecular charge transfer (ICT). Several donor units, such as phenoxazine [17] and acridine [18], are usually applied to achieve a high torsion angle between donor and acceptor units. The carbazole donor unit is also widely used for blue TADF emitters. However, a simple carbazole donor unit is insufficient because of its poor electron-donating ability and steric hindrance. In contrast, carbazole derivatives such as indolocarbazole (ICz) are promising donor units for blue TADF emitters because of their higher electron-donating ability and significant steric hindrance [19].

In this study, we developed two new TADF emitters, 3,5-bis(4-(5-phenylindolo[3,2-a]carbazole-12(5H)yl)phenyl)isonicotonitrile (ICzCN) and 2,6-bis(4-(5-phenylindolo[3,2-a]carbazole-12(5H)yl)phenyl)nicotinonitrile (ICzCYP). ICz donor and nicotinonitrile acceptor units were introduced to form twisted donor-acceptor-donor (D-A-D) molecular structures. ICzCN has symmetric D-A-D molecular structures, while ICzCYP has an asymmetric one because of the position of the introduced cyano-substituent in the acceptor unit. In this paper, we researched differences in characteristics according to symmetry from the position of the cyano-substituent in the acceptor unit.

2. Results and Discussion

2.1. Synthesis and Characterization

The synthesis procedure for obtaining ICzCN and ICzCYP is outlined in Scheme S1. The reaction was conducted in an anhydrous solvent under a nitrogen atmosphere using Suzuki Miyaura coupling reactions between 2 and 3,5-dichloroisonicotinonitrile (for ICzCN) or 2,6-dichloronicotinonitrile (for ICzCYP) [20,21]. Before measurements and device fabrication, temperature-gradient sublimation was performed to obtain high-purity materials, and the chemical structure of the final products was confirmed through $^1$H nuclear magnetic resonance (NMR) spectroscopy and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectroscopy analysis (Figure S1). Furthermore, the thermal properties of the materials were observed using differential scanning calorimetry (DSC) to measure the glass transition temperature and thermogravimetric analysis (TGA) to measure the decomposition temperature. No glass transition temperature was detected in the DSC analysis of emitters, and the decomposition temperatures of ICzCN and ICzCYP were 521 and 540 °C (Figure S3).

2.2. Density Functional Theory (DFT) Calculations

The density functional theory (DFT) calculation was executed to predict the characteristics of ICzCN and ICzCYP emitters. We confirmed that both emitters fulfill the conditions of TADF, including $\Delta E_{ST}$ below 0.3 eV, and confirmed the frontier molecular orbital contributions (FTO) and energy levels by performing time-dependent DFT (TD-DFT) calculations at the B3LYP/6-31G(d) level (Table S1). As depicted in Figure 1a, the dihedral angles between phenyl linkers and cyanopyridine ($\theta_{A-\pi}$) of ICzCN are 48° and 55°, and those of ICzCYP were 19° and 31°. Furthermore, the dihedral angles between phenyl linkers and ICz units ($\theta_{D-\pi}$) of ICzCN and ICzCYP were 50–52° and 48–50°. Because the degree of twist between the ICz units and phenyl linker was high, HOMO and LUMO were well separated from each other in both emitters, and the $\Delta E_{ST}$ values of ICzCN and ICzCYP were 0.01 and 0.03 eV. Therefore, we estimated an improvement in the up-conversion rate from the T$_1$ to the S$_1$ state [22].

We also identified dipole moments and the orientation of the optimized emitters. ICzCN and ICzCYP had a dipole moment of 3.84 and 2.43 debye, and we approximated a stronger charge transfer in ICzCN than in ICzCYP (Figure S2). Furthermore, two emitters with different cyano-substituent positions exhibited different HOMO distributions of donor units. Compared with ICzCN, where HOMO is distributed in both donors, ICzCYP exhibited only a HOMO distribution in the 3-position of the acceptor. We confirmed that these differences would produce different characteristics in the two emitters.
exhibited only a HOMO distribution in the 3-position of the acceptor. We confirmed that these differences would produce different characteristics in the two emitters.

Figure 1. Optimized chemical structures and energy levels of \( S_1 \) and \( T_1 \) states and frontier orbital distributions of (a) ICzCN and (b) ICzCYP.

2.3. Photophysical Properties

The ultraviolet-visible (UV-Vis) absorption and photoluminescence (PL) spectra of ICzCN and ICzCYP were measured in toluene. The absorption peaks (\( \lambda_{\text{abs}} \)) of the two emitters representing a broad, weak peak are 371 nm for ICzCN and 370 nm for ICzCYP because of the ICT of electrons between the donor moiety and the acceptor moiety. The maximum emission peaks (\( \lambda_{\text{PL}} \)) in toluene are 489 and 475 nm, all generating blue emissions (Figure 2). Furthermore, 12 wt% ICzCN and ICzCYP doped films in 2,8-bis(diphenylphosphineoxide)dibenzofuran (PPF) were fabricated to validate the photophysical properties of materials (Figure S7). PPF has a high \( T_1 \) energy of 3.1 eV, which prevents exciton quenching from the \( T_1 \) state of the TADF emitter to the host matrix [23].
ICzCN and ICzCYP doped film emitted sky-blue emission, with peaks of 491 and 484 nm, which were redshifted by 2 and 9 nm relative to those measured in toluene. The reason for this phenomenon is the interaction between the polar PPF host and the emitter [24]. Through measurement of the difference between the $S_1$ energy level obtained from the onset of the fluorescence spectra measured at 77 K and the $T_1$ energy level obtained from the onset of the phosphorescence spectra measured at 77 K, a small $\Delta E_{ST}$ for efficient RISC process was estimated as 0.06 eV for ICzCN and 0.05 eV for ICzCYP (Figure S5). The PL quantum yield ($\Phi_{PL}$) levels of 12 wt% ICzCN and ICzCYP doped films were measured to verify the ability of ICzCN and ICzCYP as an emitter, with values of 76 and 58% (Tables 1 and S2).

**Table 1. Photophysical properties of ICzCN and ICzCYP emitters.**

| Emitter | $\lambda_{abs}$ (nm) | $\lambda_{PL}$ [nm] | $\Phi_{PL}$ [%] | $\tau_p$ [ns/µs] | $\tau_d$ [µs/%] | $I_p/E_p/E_g$ (eV) | $E_s/E_{ST}/\Delta E_{ST}$ (eV) |
|---------|----------------------|---------------------|-----------------|-----------------|----------------|-----------------|-----------------|
| ICzCN   | 371                  | 489/491             | 63/76           | 56/30           | 14/46         | 5.80/2.93/2.87 | 2.85/2.79/0.06  |
| ICzCYP  | 370                  | 475/484             | 52/58           | 42/27           | 31/31         | 5.86/2.95/2.91 | 2.88/2.83/0.05  |

1 Measured in dilute toluene solution ($10^{-5}$ M) at room temperature. 2 12 wt% doped film in PPF matrix. 3 Transient PL decay lifetime of prompt ($\tau_p$) and delayed ($\tau_d$) fluorescence for the 12 wt% doped films measured at 300 K. 4 Fractional contribution of prompt ($\Phi_p$) and delayed ($\Phi_d$) of the 12 wt% doped film measured at 300 K. 5 $I_p$ was estimated from photoelectron yield spectroscopy, $E_a$ is electron affinity and $E_g$ was obtained by the onset of the absorption spectra of neat film. 6 $S_1$ and $T_1$ energies were obtained from the onset wavelengths in the PL spectra of 12 wt% doped films at 77 K.

The decay lifetime of the prompt and delayed components in transient PL decay curves of 12 wt% ICzCN and ICzCYP doped films at 300 K were determined by the fitted triexponential model. The TADF characteristics of both emitters in temperature-dependent PL spectra were evident at 300 K (Figure 3 and Figure S8). The prompt decay lifetime ($\tau_p$) was obtained from the nano-second scale data, and the delayed decay lifetime ($\tau_d$) was obtained from the micro-second scale data. $\tau_p$ was 56 ns for ICzCN and 42 ns for ICzCYP, and $\tau_d$ was 14 µs for ICzCN and 31 µs for ICzCYP. The delayed decay lifetime of ICzCYP is longer than that of ICzCN, depending on the different positions of the cyano-substituent.
Molecules 2022, 27, x FOR PEER REVIEW 5 of 8

Figure 3. Temperature-dependent transient PL decay curves of (a) 12 wt% ICzCN:PPF and (b) ICzCYP:PPF doped films.

Furthermore, both emitters have a larger $\Phi_d$ than $\Phi_p$ because $k_{\text{ISC}}$ is much larger than $k_d$. ICzCN achieved a high $\Phi_{\text{RISC}}$ of 84% compared with ICzCYP because ICzCN achieved a competitive $k_{\text{RISC}}$ ratio to $k_{\text{RISC}}$ given its small $k_{\text{RISC}}$ value of $4.4 \times 10^5$ s$^{-1}$ [25,26]. The HOMO energy level also differed because of the position of the cyano-substituent group in the molecule. The ionization energy ($E_{\text{i}}$) obtained by photoelectron yield spectroscopy of neat film was 5.80 eV for ICzCN and 5.86 eV for ICzCYP, which affected the contribution of the donor based on the cyano-substituent position in emitters (Figures S4 and S6).

Moreover, all rate constants values except $k_{\text{RISC}}$ were greater than those of ICzCYP because of the smaller $\tau_p$, $\tau_d$ of ICzCN. The $k_{\text{RISC}}$ was larger in ICzCN because of the structure in which both donors are located at the ortho-position of the cyano-substituent and the higher $\Phi_d$ to $\Phi_p$ ratio of ICzCN than ICzCYP [27,28]. Detailed rate constants are presented in Table 2, and the equation-of-rate constants are displayed in Supplementary Materials.

Table 2. Photophysical properties of 12 wt% ICzCN:PPF and ICzCYP:PPF doped film.

| Emitter | $k^5_d$ (s$^{-1}$) | $k_d$ (s$^{-1}$) | $k_{\text{RISC}}$ (s$^{-1}$) | $k_{\text{ISC}}$ (s$^{-1}$) | $\Phi_{\text{ISC}}$ (%) | $\Phi_{\text{RISC}}$ (%) |
|---------|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| ICzCN   | 1.3 × 10$^7$     | 1.3 × 10$^5$    | 4.4 × 10$^4$    | 3.0 × 10$^7$    | 2.8 × 10$^5$    | 54              | 84              |
| ICzCYP  | 6.7 × 10$^6$     | 1.1 × 10$^5$    | 6.4 × 10$^4$    | 1.8 × 10$^7$    | 1.8 × 10$^5$    | 69              | 45              |

2.4. Electroluminescence (EL) Performance

For measuring the electroluminescence (EL) performance of ICzCN and ICzCYP as TADF emitters, a device composed of indium tin oxide (ITO)/1,4,5,7,8,11-hexaazatriphenylene-hexacarbonitrile (HATCN), 10 nm/NN,N'-di(1-naphthyl)-N,N'-diphenyl-(1,1'-biphenyl)-4,4'-diamine (α-NPD, 30 nm)/1,3-bis(N-carbazolyl)benzene (mCP, 5 nm)/12 wt% ICzCN:PPF or ICzCYP:PPF emitter (30 nm)/PPF (5 nm)/2,2',2''-(1,3,5-benzinetrizyl)-tris(1-phenyl-1-$H$-benzimidazole (TPBi, 40 nm)/Lithium fluoride (LiF, 0.8 nm)/Aluminum (Al, 80 nm) was fabricated. In this structure, we used HATCN as a hole-injection layer (HIL), and α-NPD and TPBi as the hole-transporting layer (HTL) and electron-transporting layer (ETL). Furthermore, mCP and PPF served as exciton-blocking layers to prohibit $T_1$ exciton quenching from the emitting layer to the hole-electron transporting layer [29].

The energy-level diagram of the TADF-OLEDS device of ICzCN and ICzCYP is confirmed in Figure 4a. The emission wavelength of devices in the EL spectra were 507 nm for ICzCN emitting green light and 497 nm for ICzCYP emitting sky-blue light (Figure 4b). The current-density-voltage-luminance ($J$-$V$-$L$) characteristics and external quantum efficiency (EQE, $\eta_{\text{ext}}$) versus luminance of devices for ICzCN and ICzCYP are indicated in Figure 4c,d. These devices achieved low turn-on voltage ($V_{\text{on}}$) of less than 3.4 $V$, and the maximum luminance ($L_{\text{max}}$) values are 13742 cd m$^{-2}$ for ICzCN and 7627 cd m$^{-2}$ for ICzCYP. Furthermore, the reduction of EQE values compared with maximum $\eta_{\text{ext}}$ was
observed at 100 and 1000 cd m\(^{-2}\), and roll-off efficiencies were 23 and 43% for the device with ICzCN emitter and 55 and 81% for the device with ICzCYP. ICzCN achieved a high \(k_{\text{RISC}}\) value of \(1.8 \times 10^5\) s\(^{-1}\), which enabled efficient \(T_1\) exciton transfer and suppressed roll-off of device. While ICzCYP suffers from severe high roll-off efficiency because of the strong \(T_1\) exciton annihilation process attributed to the longer \(T_1\) exciton lifetime compare with ICzCN [30]. EL performance data of the devices are presented in Table 3.

![Figure 4](image-url)

**Figure 4.** (a) Energy level diagram of a TADF-OLEDs device with ICzCN and ICzCYP as an emitter. (b) EL spectra of 12 wt% ICzCN and ICzCYP devices at 10 mA cm\(^{-2}\). (c) Current density-voltage-luminance (J-V-L) curves of TADF-OLEDs device with 12 wt% ICzCN and ICzCYP applied as emitter. (d) External quantum efficiency versus luminance (\(\eta_{\text{ext}}\)) of devices.

### Table 3. EL performance data of 12 wt% ICzCN and ICzCYP devices.

| Emitter | \(\lambda_{\text{EL}}\) (nm) | \(V_{\text{on}}\) (V) | \(L_{\text{max}}\) (cd m\(^{-2}\)) | \(\eta_c\) (cd A\(^{-1}\)) | \(\eta_p\) (lm W\(^{-1}\)) | \(\eta_{\text{ext}}\) (%) | CIE\(_{x,y}\) \(\text{ Commission Internationale de l’Éclairage (CIE) color coordination.} \)
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| ICzCN   | 507             | 3.4             | 13742           | 42.1            | 44.1            | 14.8            | (0.26, 0.47)    |
| ICzCYP  | 497             | 3.3             | 7627            | 46.5            | 50.3            | 14.9            | (0.23, 0.45)    |

\(^1\) Maximum emission peak in EL spectra. \(^2\) Turn-on voltage of devices at 1 cd m\(^{-2}\). \(^3\) Maximum current efficiency (\(\eta_c\)), maximum power efficiency (\(\eta_p\)), and external quantum efficiency (\(\eta_{\text{ext}}\)) \(^4\) Commission Internationale de l’Éclairage (CIE) color coordination.

### 3. Conclusions

In this study, we developed ICzCN and ICzCYP based on pyridinecarbonitrile and ICz as TADF emitters with symmetry and asymmetry of the acceptor unit according to the position change of the cyano-substituent. Both emitters exhibited small \(\Delta E_{\text{ST}}\) values of 0.06 and 0.05 eV from effective HOMO and LUMO separation. ICzCN achieved a high \(\Phi_{\text{RISC}}\) of 84% from a small \(k_{\text{RISC}}\) of \(4.4 \times 10^4\) s\(^{-1}\), large \(k_{\text{RISC}}\) of \(2.8 \times 10^5\) s\(^{-1}\), and \(\kappa_{\text{ISC}}\) of \(3.0 \times 10^2\) s\(^{-1}\), enabling efficient \(T_1\) exciton harvesting. Furthermore, devices realized a maximum \(\eta_{\text{ext}}\) of 14.8% for ICzCN and 14.9% for ICzCYP in green and sky-blue light emission. Based on these results, we confirmed the electron-accepting substituent position...
Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/molecules27238274/s1, Scheme S1: Synthesis of ICzCN and ICzCYP. Figure S1: $^1$H NMR of (a) 1, (b) 2, (c) ICzCN and (d) ICzCYP. Table S1: $T_1$ and $S_1$ excitation energies (vertical transition), oscillator strength ($f$), and transition configurations of the nicotinonitrile derivatives ICzCN and ICzCYP calculated by TD-DFT at the B3LYP/6-31G(d). Figure S2: The transition dipole moments of (a) ICzCN and (b) ICzCYP in optimized molecular structure. Figure S3: TGA profiles of ICzCN (black) and ICzCYP (red). Figure S4: Photoelectron yield spectra of (a) ICzCN and (b) ICzCYP. Figure S5: PL spectra of prompt fluorescence at 300 K (black), phosphorescence at 77 K (red) for (a) ICzCN and (b) ICzCYP and fluorescence (black) and phosphorescence (red) at 77 K for (c) ICzCN and (d) ICzCYP. Figure S6: UV-Vis and PL spectra of (a) ICzCN and (b) ICzCYP neat films. Figure S7: PL spectra of 12 wt% (a) ICzCN and (b) ICzCYP doped films in PPF host. Figure S8: Streak images and time-resolved PL spectra of 12 wt% (a) ICzCN:PPF and (b) ICzCYP:PPF co-deposited films. Table S2: Photophysical properties of ICzCN and ICzCYP in solution, neat film and 12 wt% doped film in PPF host [12,20,21,31].

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Sample Availability: Samples of the compounds ICzCN and ICzCYP are available from the authors.

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