Supporting Information

Efficient blue electroluminescence with external quantum efficiency of 9.20% and CIE_y < 0.08 without excimer emission

Jayaraman Jayabharathi*, Sekar Sivaraj, Venugopal Thanikachalam, Balu Seransenguttuvan
Department of Chemistry, Annamalai University, Annamalainagar, Tamilnadu- 608 002, India,
Email: jitchalam2005@yahoo.co.in

Address for correspondence

Dr. J. Jayabharathi
Professor of Chemistry
Department of Chemistry
Annamalai University
Annamalai nagar 608 002
Tamilnadu, India.
Tel: +91 9443940735
E-mail:jitchalam2005@yahoo.co.in
Contents:

SI-I: Scheme S1

SI-II: Spectra of emissive materials (Schemes S2-S5)

SI-III: Figures S1 (a) AFM images; (b) Favoured and unfavoured configurations of blue emitters

SI-IV: Solvatochromism: Figures S2- S4

SI-V: Charge-Transfer Intexes

SI-VI: Natural Transition Orbitals: Figures S5 - S7

SI-VII: Hole-Particle Distribution: Figures S8 - S10

SI-VIII: Potential Energy Scan (PES): Figures S11

SI-IX: Tables S1-S15
SI-I: Scheme S1. Synthetic route of emissive materials
SI-II: Spectra of emissive materials (Schemes S2-S4)

Scheme S2. Spectra of (a) PPI-Cz; (b) PPICN-Cz
Scheme S3. Spectra of (a) PPI-Py; (b) PPICN-Py
Scheme S4. Spectra of (a) PPI-An; (b) PPICN-An
Scheme S5. Spectra of (a)PPI-Cz; (b) PPICN-Cz; (c)PPI-Py; (d) PPICN-Py; (e)PPI-An; (f) PPICN-An.
SI-III: Figure S1 (a) AFM images; (b) Favoured and unfavoured configurations of blue emitters
SI-IV: Solvatochromism (Figures S2-S4):

**Figure S2.** Absorption spectra of emissive materials.
**Figure S3.** Emission spectra of emissive materials.

**SI-V: Figure S4.** Lippert - Mataga plot.
SI–V: Charge-Transfer Intexes

The hole-particle pair interactions have been related to the distance covered during the excitations one possible descriptor $\Delta r$ index could be used to calculate the average distance which is weighted in function of the excitation coefficients.

\[
\Delta r = \frac{\sum_{ia} k_i^2 |\langle \varphi_a | r | \varphi_a \rangle - \langle \varphi_i | r | \varphi_i \rangle|}{\sum_{ia} k_i^2} \quad \text{............... (S1)}
\]

Where $|\langle \varphi_i | r | \varphi_i \rangle|$ is the norm of the orbital centroid [1–4] and $\Delta r$ index will be expressed in Å.

The density variation associated to the electronic transition is given by

\[
\Delta \rho(r) = \rho_{EX}(r) - \rho_{GS}(r) \quad \text{............... (S2)}
\]

Where $\rho_{GS}(r)$ and $\rho_{EX}(r)$ are the electronic densities of to the ground and excited states, respectively. Two functions, $\rho_+(r)$ and $\rho_-(r)$, corresponds to the points in space where an increment or a depletion of the density upon absorption is produced and they can be defined as follows:

\[
\rho_+(r) = \begin{cases} 
\Delta \rho(r) & \text{if } \Delta \rho(r) > 0 \\
0 & \text{if } \Delta \rho(r) < 0 
\end{cases} \quad \text{............... (S3)}
\]

\[
\rho_-(r) = \begin{cases} 
\Delta \rho(r) & \text{if } \Delta \rho(r) < 0 \\
0 & \text{if } \Delta \rho(r) > 0 
\end{cases} \quad \text{............... (S4)}
\]

The barycenters of the spatial regions $R_+$ and $R_-$ are related with $\rho_+(r)$ and $\rho_-(r)$ and are shown as

\[
R_+ = \frac{\int r \rho_+(r) dr}{\int \rho_+(r) dr} = (x_+, y_+, z_+) \quad \text{............... (S5)}
\]

\[
R_- = \frac{\int r \rho_-(r) dr}{\int \rho_-(r) dr} = (x_-, y_-, z_-) \quad \text{............... (S6)}
\]
The spatial distance \( D_{CT} \) between the two barycenters \( R_+ \) and \( R_- \) of density distributions can thus be used to measure the CT excitation length

\[
D_{CT} = \left| R_+ - R_- \right| \quad \text{(S7)}
\]

The transferred charge \( q_{CT} \) can be obtained by integrating over all space \( \rho^+ + (\rho^-) \). Variation in dipole moment between the ground and the excited states \( (\mu_{CT}) \) can be computed by the following relation:

\[
\|\mu_{CT}\| = D_{CT} \int \rho^+ (r) dr = D_{CT} \int \rho^- (r) dr \quad \text{.......................... (S8)}
\]

\[
= D_{CT} q_{CT} \quad \text{.......................... (S9)}
\]

The difference between the dipole moments \( \|\mu_{CT}\| \) have been computed for the ground and the excited states \( \Delta\mu_{ES-GS} \). The two centroids of charges \( (C^+/C^-) \) associated to the positive and negative density regions are calculated as follows. First the root-mean-square deviations along the three axis \( (\sigma_{aj}, j = x, y, z; a = + \text{ or } -) \) are computed as

\[
\sigma_{a,j} = \sqrt{\frac{\sum \rho_a(r_i)(j_i - j_a)^2}{\sum \rho_a(r_i)}} \quad \text{.................. (S10)}
\]

The two centroids \( (C_+ \text{ and } C_-) \) are defined as

\[
C_+(r) = A_+ e^{\left( \frac{(x - x_+)^2}{2\sigma_{x+}^2} - \frac{(y - y_+)^2}{2\sigma_{y+}^2} - \frac{(z - z_+)^2}{2\sigma_{z+}^2} \right)} \quad \text{.................. (S11)}
\]

\[
C_-(r) = A_- e^{\left( \frac{(x - x_-)^2}{2\sigma_{x-}^2} - \frac{(y - y_-)^2}{2\sigma_{y-}^2} - \frac{(z - z_-)^2}{2\sigma_{z-}^2} \right)} \quad \text{.................. (S12)}
\]

The normalization factors \( (A_+ \text{ and } A_-) \) are used to impose the integrated charge on the centroid to be equal to the corresponding density change integrated in the whole space.
\[ A_+ = \frac{\int \rho_+(r)dr}{\int e^{-\left(\frac{(x-x_\perp)^2}{2\sigma_{+x}^2} + \frac{(y-y_\perp)^2}{2\sigma_{+y}^2} + \frac{(z-z_\perp)^2}{2\sigma_{+z}^2}\right)}dr} \] ........................ (S13)

\[ A_- = \frac{\int \rho_-(r)dr}{\int e^{-\left(\frac{(x-x_\perp)^2}{2\sigma_{-x}^2} + \frac{(y-y_\perp)^2}{2\sigma_{-y}^2} + \frac{(z-z_\perp)^2}{2\sigma_{-z}^2}\right)}dr} \] ........................ (S14)

H index is defined as half of the sum of the centroids axis along the D–A direction, if the D–A direction is along the X axis, H is defined by the relation:

\[ H = \frac{\sigma_{+x} + \sigma_{-x}}{2} \] ........................ (S15)

The centroid along X axis is expected. The t index represents the difference between D\textsubscript{CT} and H:

\[ t = D\textsubscript{CT} - H \] ........................ (S16)

**SI-VI: Natural Transition Orbitals (NTOs)**

The excited-state properties were examined to gain a deep insight into the intrinsic photophysics of these materials. Both natural transition orbital (NTO) and electron-hole pair wavefunction were used to describe the excited state character. The HONTOs and LUNTOs of PPI-Cz, PPICN-Cz, PPI-An, PPICN-An, PPI-Py and PPICN-Py (Figures S5-S7: Tables S7- S9) exhibit a hybrid splitting state character from interstate coupling of LE and CT levels. The % CT increases as increasing the aromatic fragment size and also partially influenced by steric hindrance. The increasing % LE in S\textsubscript{1} state enhances the photoluminance efficiency (\(\eta_{PL}\)).

Thus, compared with N-phenylcarbazole and anthracene substituted phenantrimidazole, PPI-Py and PPICN-Py exhibits high photoluminance efficiency (\(\eta_{PL}\)), high exciton utilisation efficiency (\(\eta_{S}\)) and high external quantum efficiency (\(\eta_{EQE}\)) as a result of increased LE component in S\textsubscript{1} state.
**Figure S5.** Natural transition orbital pairs (HONTOs and LUNTOs) with transition character analysis of PPI-Cz and PPICN-Cz.

**Figure S6.** Natural transition orbital pairs (HONTOs and LUNTOs) with transition character analysis of PPI-An and PPICN-An.
**Figure S7.** Natural transition orbital pairs (HONTOs and LUNTOs) with transition character analysis for singlet states of PPI-Py and PPICN-Py.

**SI-VII: Hole-Particle Distribution**

The integral of hole (h^+) and electron (e^-) of these materials with transition density is shown in Figures S8-S10. The integral overlap of hole-electron (Tables S10-S15) distribution (S) is a measure of spatial separation of hole and electron. The integral overlap (S) of hole and electron and distance (D) between centroids of hole and electron confirmed the existence of LE and CT states. Compared to parent compounds, these emitters has small D and high S value, however, The small D and high S of cyano phenanthroimidazoles on comparison to parent indicates charge transfer is higher in percentage in cyano phenanthroimidazoles. The variation of dipolemoment with respect to S_0 is outputted which is directly evaluated based on the position of centroid of hole and electron. RMSD of hole or electron characterizes their distribution breadth:
RMSD of both electron and hole in PPI-Py/ PPICN-Py and PPI-Cz/ PPICN-Cz is higher in X direction, indicates electron and hole distribution is much broader in X direction whereas RMSD of electron in PPI-An/ PPICN-An is higher in Y direction, indicates electron and hole distribution is much broader in Y direction. The H index (half sum of the axis of anisotropic density variation distribution) measures the spread of positive and negative regions related to CT. The CT index, i.e., $\iota$ index is another measure of separation of hole-electron (equations S15 and S16; Tables S10-S12). For both CADPPI and TPNCN-TPA, $\iota$ is negative in all directions which reveal that the overlap of hole and electron is severe (Figure S8). This is further evidenced by $\Delta r$ index (equation S1) which is average of hole -electron distance ($d_{h^+e^-}$) upon excitation which shows the nature of excitation type, LE or CT: valence excitation (LE) is related to short distance ($< d_{h^+e^-}$) while the larger distance ($> d_{h^+e^-}$) is related to CT excitation.
Figure S8. Hole and particle distribution of PPI-Cz and PPICN-Cz.
Figure S9. Hole and particle distribution of PPI-An and PPICN-An
**Figure S10.** Hole and particle distribution of PPI-Py and PPICN-Py
SI-VIII: Potential Energy Scan (PES)

The potential energy surfaces (PES) have been plotted as a function of twist angle between C2 substituent and phenanthroimidazole core in gas phase (Figure S11). During calculation all geometrical parameters were simultaneously relaxed while torsional angles were varied in steps of 0°, 20°, 40°, 60°….360°. Tuning the substituent at C6/C9 positions have small influence on twist angles between phenanthroimidazole plane and naphthyl group and much larger variation in θ3 and θ4 angle (θ1-PPI and C-coupling; θ2-PPI and N-coupling; θ3-C6 and PPI; θ4-C9 and PPI-N-coupling). The synthesized emitters show more twisted configuration (θ1~25°; θ2~75°; θ3~55°; θ4~56.0°) due to larger steric hindrance between the substituent with phenanthroimidazole core. The non-coplanar twisted conformation can effectively suppress the molecular aggregation, the almost orthogonal dihedral angles (~89.0°) between N-coupling and phenanthroimidazole core effectively minimize the intermolecular packing and used as hole-trapping sites whereas peripheral phenanthroimidazole core blocks electron-trapping sites. Thus, effective carrier injection as well as transport ability will be expected from these reported emitter and the relative charge carrier transport ability of the title materials was investigated by hole-only devices as well as electron-only devices. The introduction of C6/C9 substituents on phenanthroimidazole unit could enhance the molecular distortion degree, thereby suppress the formation of aggregation or π-π stacking in the solid state and form amorphous film during device fabrication The non-planar conformation may effectively suppresses red shift and maintains quantum efficiency in film via restraining intermolecular interaction. The incorporation of bulky fragments at C6/C9 positions and side capping into phenanthroimidazoles enlarged the size and improved their thermal stability.
Figure S11. Potential energy surface scan (PES) diagram of emissive materials.
**Table S1**: Photophysical properties of PPI-Cz in different solvents.

| Solvents | ε   | n   | f(ε,n) | λ<sub>ab</sub> (nm) | υ<sub>ab</sub> (cm⁻¹) | λ<sub>flu</sub> (nm) | υ<sub>flu</sub> (cm⁻¹) | υ<sub>ss</sub> (cm⁻¹) | ΔG (kcal/mol) | Δ(ΔG<sub>hex</sub>−ΔG<sub>sol</sub>) (kcal/mol) | λ (kcal/mol) |
|----------|-----|-----|--------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------|---------------------------------|-------------|
| hexane   | 2.42| 1.401| 0.048  | 278                 | 34482.76            | 372                 | 24271.84            | 10210.91           | 83.98         | 8.15                            | 14.59       |
| dioxane  | 3.39| 1.474| 0.0878 | 280                 | 34246.58            | 375                 | 24038.46            | 10653.57           | 83.55         | 8.03                            | 14.66       |
| CCl₄     | 3.08| 1.399| 0.096  | 283                 | 34364.26            | 381                 | 24271.84            | 10092.42           | 83.81         | 8.32                            | 14.42       |
| benzene  | 4.33| 1.352| 0.1669 | 285                 | 34602.08            | 383                 | 24271.84            | 10330.23           | 84.15         | 7.98                            | 14.76       |
| chloroform | 6.09| 1.4131| 0.186569 | 287                 | 34602.08            | 386                 | 24038.46            | 10563.61           | 83.81         | 8.31                            | 15.10       |
| ethyl acetate | 7.52| 1.405| 0.209634 | 289                 | 34364.26            | 391                 | 23980.82            | 10383.45           | 83.39         | 8.73                            | 14.84       |
| THF      | 9.08| 1.4242| 0.218349 | 290                 | 34129.69            | 395                 | 25000              | 9129.693           | 84.51         | 7.61                            | 13.05       |
| dichloromethane | 36.7| 1.427| 0.276  | 293                 | 34722.22            | 400                 | 25062.66            | 9659.566           | 85.45         | 6.67                            | 13.80       |
| acetonitrile | 37.5| 1.3442| 0.305378 | 295                 | 34364.26            | 40                  | 24330.9            | 10033.36           | 83.89         | 8.23                            | 14.34       |
Table S2: Photophysical properties of PPI-CN-Cz in different solvents.

| Solvents   | ε   | n   | f(ε,n) | ET(30) | λ<sub>ab</sub> (nm) | ν<sub>ab</sub> (cm<sup>-1</sup>) | λ<sub>flu</sub> (nm) | ν<sub>flu</sub> (cm<sup>-1</sup>) | ν<sub>ss</sub> (cm<sup>-1</sup>) | ΔG (kcal/mol) | Δ(ΔG<sub>hex</sub>-ΔG<sub>sol</sub>) (kcal/mol) | λ (kcal/mol) |
|------------|-----|-----|--------|--------|----------------------|------------------------|----------------------|------------------------|----------------------|--------------|---------------------------------------------|------------|
| hexane     | 1.88| 1.37| 0.000411| 32.4   | 269                  | 44052.86               | 375                  | 24752.48               | 19300.39             | 98.34        | -15.82                                      | 27.59      |
| dioxane    | 2.22| 1.42| 0.021437| 36.0   | 273                  | 43103.45               | 379                  | 24449.88               | 18653.57             | 96.55        | -14.03                                      | 26.66      |
| CCl<sub>4</sub> | 2.23| 1.46| 0.011075| 39.1   | 275                  | 41841.00               | 383                  | 24038.46               | 17802.54             | 94.16        | -11.64                                      | 25.44      |
| benzene    | 2.28| 1.42| 0.026639| 34.3   | 278                  | 41152.26               | 385                  | 23696.68               | 17455.58             | 92.69        | -10.17                                      | 24.95      |
| chloroform | 4.81| 1.44| 0.148262| 39.1   | 280                  | 40322.58               | 388                  | 23041.47               | 17281.11             | 90.56        | -8.04                                       | 24.70      |
| ethyl acetate | 6.09| 1.41| 0.186569| 38.1   | 282                  | 40000.00               | 390                  | 22573.36               | 17426.64             | 89.43        | -6.91                                       | 24.91      |
| THF        | 7.52| 1.40| 0.209634| 37.4   | 284                  | 39062.50               | 393                  | 22026.43               | 17036.07             | 87.31        | -4.79                                       | 24.35      |
| dichloromethane | 9.08| 1.42| 0.218349| 40.7   | 286                  | 40322.58               | 398                  | 21739.13               | 18583.45             | 88.70        | -6.18                                       | 26.56      |
| acetonitrile | 37.5| 1.34| 0.305378| 45.6   | 288                  | 38759.69               | 405                  | 21459.23               | 17300.46             | 86.07        | -3.55                                       | 24.73      |
Table S3: Photophysical properties of PPI- An in different solvents.

| Solvents | $\varepsilon$ | $n$ | $f(\varepsilon,n)$ | ET(30) | $\lambda_{ab}$ (nm) | $\nu_{ab}$ (cm$^{-1}$) | $\lambda_{flu}$ (nm) | $\nu_{flu}$ (cm$^{-1}$) | $\nu_{ss}$ (cm$^{-1}$) | $\Delta G$ (kcal/mol) | $\Delta(\Delta G_{hex}-\Delta G_{sol})$ (kcal/mol) | $\lambda$ (kcal/mol) |
|----------|-------|-----|-----------------|--------|-----------------|--------------------|-----------------|--------------------|--------------------|-----------------|-----------------------------------------------|-----------------|
| hexane   | 1.88  | 1.37 | 0.000411        | 32.4   | 226             | 43103.45           | 381             | 24330.9            | 18772.55          | 96.38           | -13.86                                               | 26.83           |
| dioxane  | 2.22  | 1.42 | 0.021437        | 36.0   | 228             | 42194.09           | 385             | 24038.46           | 18155.63          | 94.66           | -12.14                                               | 25.95           |
| CCl$_4$  | 2.23  | 1.46 | 0.011075        | 39.1   | 231             | 41322.31           | 388             | 23752.97           | 17569.34          | 93.01           | -10.49                                               | 25.11           |
| benzene  | 2.28  | 1.42 | 0.026639        | 34.3   | 233             | 41152.26           | 391             | 23364.49           | 17787.78          | 92.21           | -9.69                                                 | 25.42           |
| chloroform | 4.81  | 1.44 | 0.148262        | 39.1   | 235             | 40485.83           | 395             | 22988.51           | 17497.32          | 90.72           | -8.20                                                 | 25.01           |
| ethyl acetate | 6.09  | 1.41 | 0.186569        | 38.1   | 236             | 40160.64           | 398             | 22727.27           | 17433.37          | 89.88           | -7.36                                                 | 24.92           |
| THF      | 7.52  | 1.40 | 0.209634        | 37.4   | 238             | 40000.00           | 400             | 22421.52           | 17578.48          | 89.22           | -6.70                                                 | 25.12           |
| dichloromethane | 9.08  | 1.42 | 0.218349        | 40.7   | 240             | 40322.58           | 403             | 21739.13           | 18583.45          | 88.70           | -6.18                                                 | 26.56           |
| acetonitrile | 37.5  | 1.34 | 0.305378        | 45.6   | 245             | 39062.5            | 406             | 22172.95           | 16889.55          | 87.52           | -5.00                                                 | 24.14           |
Table S4: Photophysical properties of PPI-CN-An in different solvents.

| Solvents     | ε     | n     | f(ε,n) | ET(30) | λ<sub>ab</sub> (nm) | v<sub>ab</sub> (cm<sup>-1</sup>) | λ<sub>flu</sub> (nm) | v<sub>flu</sub> (cm<sup>-1</sup>) | v<sub>ss</sub> (cm<sup>-1</sup>) | ΔG (kcal/mol) | Δ(ΔG<sub>hex</sub>-ΔG<sub>sol</sub>) (kcal/mol) | λ (kcal/mol) |
|--------------|-------|-------|--------|--------|------------------|----------------|-------------|----------------|----------------|--------------|--------------------------------|--------------|
| hexane       | 1.88  | 1.37  | 0.000411 | 32.4  | 231              | 44052.86       | 374         | 24752.48       | 19300.39       | 98.34        | -15.82                                | 27.59        |
| dioxane      | 2.22  | 1.42  | 0.021437 | 36.0  | 232              | 43103.45       | 378         | 24449.88       | 18653.57       | 96.55        | -14.03                                | 26.66        |
| CCl<sub>4</sub> | 2.23  | 1.46  | 0.011075 | 39.1  | 235              | 41841.00       | 380         | 24038.46       | 17802.54       | 94.16        | -11.64                                | 25.44        |
| benzene      | 2.28  | 1.42  | 0.026639 | 34.3  | 237              | 41152.26       | 382         | 23696.68       | 17455.58       | 92.69        | -10.17                                | 24.95        |
| chloroform   | 4.81  | 1.44  | 0.148262 | 39.1  | 238              | 40322.58       | 384         | 23041.47       | 17281.11       | 90.56        | -8.04                                 | 24.70        |
| ethyl acetate| 6.09  | 1.41  | 0.186569 | 38.1  | 240              | 40000.00       | 388         | 22573.36       | 17426.64       | 89.43        | -6.91                                 | 24.91        |
| THF          | 7.52  | 1.40  | 0.209634 | 37.4  | 242              | 39062.50       | 390         | 22026.43       | 17036.07       | 87.31        | -4.79                                 | 24.35        |
| dichloromethane | 9.08  | 1.42  | 0.218349 | 40.7  | 245              | 40322.58       | 393         | 21739.13       | 18583.45       | 88.70        | -6.18                                 | 26.56        |
| acetonitrile | 37.5  | 1.34  | 0.305378 | 45.6  | 250              | 38759.69       | 396         | 21459.23       | 17300.46       | 86.07        | -3.55                                 | 24.73        |
| Solvents       | ε    | n    | f(ε,n) | ET(30) | λ<sub>ab</sub> (nm) | v<sub>ab</sub> (cm<sup>-1</sup>) | λ<sub>flu</sub> (nm) | v<sub>flu</sub> (cm<sup>-1</sup>) | v<sub>ss</sub> (cm<sup>-1</sup>) | ΔG (kcal/mol) | Δ(ΔG<sub>hex</sub>−ΔG<sub>sol</sub>) (kcal/mol) | λ (kcal/mol) |
|---------------|------|------|--------|--------|---------------------|-------------------------|---------------------|-----------------|-----------------|--------------|--------------------------------------------------|-------------|
| hexane        | 1.88 | 1.37 | 0.000411 | 32.4  | 327                 | 43103.45                | 405                 | 24330.9         | 18772.55        | 96.38        | -13.86                                            | 26.83       |
| dioxane       | 2.22 | 1.42 | 0.021437 | 36.0  | 328                 | 42194.09                | 410                 | 24038.46         | 18155.63        | 94.66        | -12.14                                            | 25.95       |
| CCl<sub>4</sub> | 2.23 | 1.46 | 0.011075 | 39.1  | 331                 | 41322.31                | 415                 | 23752.97         | 17569.34        | 93.01        | -10.49                                            | 25.11       |
| benzene       | 2.28 | 1.42 | 0.026639 | 34.3  | 333                 | 41152.26                | 419                 | 23364.49         | 17787.78        | 92.21        | -9.69                                             | 25.42       |
| chloroform    | 4.81 | 1.44 | 0.148262 | 39.1  | 335                 | 40485.83                | 423                 | 22988.51         | 17497.32        | 90.72        | -8.20                                             | 25.01       |
| ethyl acetate | 6.09 | 1.41 | 0.186569 | 38.1  | 336                 | 40160.64                | 425                 | 22727.27         | 17433.37        | 89.88        | -7.36                                             | 24.92       |
| THF           | 7.52 | 1.40 | 0.209634 | 37.4  | 339                 | 40000                   | 428                 | 22421.52         | 17578.48        | 89.22        | -6.70                                             | 25.12       |
| dichloromethane| 9.08 | 1.42 | 0.218349 | 40.7  | 342                 | 40322.58                | 430                 | 21739.13         | 18583.45        | 88.70        | -6.18                                             | 26.56       |
| acetonitrile  | 37.5 | 1.34 | 0.305378 | 45.6  | 345                 | 39062.5                 | 435                 | 22172.95         | 16889.55        | 87.52        | -5.00                                             | 24.14       |
### Table S6: Photophysical properties of PPI-CN-Py in different solvents.

| Solvents   | $\epsilon$ | $n$  | $f(\epsilon,n)$ | ET(30) | $\lambda_{ab}$ (nm) | $\nu_{ab}$ (cm$^{-1}$) | $\lambda_{flu}$ (nm) | $\nu_{flu}$ (cm$^{-1}$) | $\nu_{ss}$ (cm$^{-1}$) | $\Delta G$ (kcal/mol) | $\Delta(\Delta G_{\text{hex}}-\Delta G_{\text{sol}})$ (kcal/mol) | $\lambda$ (kcal/mol) |
|------------|------------|------|------------------|--------|----------------------|-------------------------|---------------------|-------------------------|------------------------|---------------------|---------------------------------------------------------------|---------------------|
| hexane     | 1.88       | 1.37 | 0.000411         | 32.4   | 326                  | 44052.86                | 405                 | 24752.48                | 19300.39               | 98.34               | -15.82                                                        | 27.59               |
| dioxane    | 2.22       | 1.42 | 0.021437         | 36.0   | 328                  | 43103.45                | 410                 | 24449.88                | 18653.57               | 96.55               | -14.03                                                        | 26.66               |
| CCl$_4$    | 2.23       | 1.46 | 0.011075         | 39.1   | 330                  | 41841.00                | 413                 | 24038.46                | 17802.54               | 94.16               | -11.64                                                        | 25.44               |
| benzene    | 2.28       | 1.42 | 0.026639         | 34.3   | 332                  | 41152.26                | 415                 | 23696.68                | 17455.58               | 92.69               | -10.17                                                        | 24.95               |
| chloroform | 4.81       | 1.44 | 0.148262         | 39.1   | 334                  | 40322.58                | 419                 | 23041.47                | 17281.11               | 90.56               | -8.04                                                         | 24.70               |
| ethyl acetate | 6.09   | 1.41 | 0.186569         | 38.1   | 337                  | 40000.00                | 420                 | 22573.36                | 17426.64               | 89.43               | -6.91                                                         | 24.91               |
| THF        | 7.52       | 1.40 | 0.209634         | 37.4   | 338                  | 39062.50                | 422                 | 22026.43                | 17036.07               | 87.31               | -4.79                                                         | 24.35               |
| dichloromethane | 9.08 | 1.42 | 0.218349         | 40.7   | 340                  | 40322.58                | 425                 | 21739.13                | 18583.45               | 88.70               | -6.18                                                         | 26.56               |
| acetonitrile | 37.5   | 1.34 | 0.305378         | 45.6   | 343                  | 38759.69                | 429                 | 21459.23                | 17300.46               | 86.07               | -3.55                                                         | 24.73               |
Table S7: Computed excitation energy (eV), excitation coefficient, $\Delta r$ (Å), oscillator strength ($f$) and dipole moment ($\mu$, D) for singlet states of PPI-Cz and PPICN-Cz.

| Emitters     | State | Excitation energy | Excitation coefficient | $\Delta r$ | Oscillator strength | $\mu$ | NTO Transitions |
|--------------|-------|-------------------|------------------------|------------|---------------------|------|-----------------|
| PPI-Cz       | 1     | 3.44              | 0.3599                 | 2.5807     | 0.0940              | 0.80 | 170 $\rightarrow$ 174 |
|              | 2     | 3.50              | 0.3496                 | 2.0300     | 0.1217              | 0.52 | 169 $\rightarrow$ 171 |
|              | 3     | 3.53              | 0.3984                 | 2.4008     | 0.5972              | 1.20 | 170 $\rightarrow$ 172 |
|              | 4     | 3.66              | 0.3806                 | 4.0709     | 0.0216              | 0.50 | 169 $\rightarrow$ 178 |
|              | 5     | 3.83              | 0.3534                 | 1.9721     | 0.0526              | 1.43 | 170 $\rightarrow$ 176 |
| PPICN-Cz     | 1     | 0.55              | 0.47062                | 1.1576     | 0.0067              | 3.10 | 172 $\rightarrow$ 175 |
|              | 2     | 0.61              | 0.48113                | 1.0686     | 0.0008              | 1.66 | 173 $\rightarrow$ 178 |
|              | 3     | 0.84              | 0.45874                | 1.4100     | 0.0081              | 2.79 | 174 $\rightarrow$ 178 |
|              | 4     | 1.57              | 0.42863                | 1.2663     | 0.0603              | 1.87 | 170 $\rightarrow$ 175 |
|              | 5     | 1.59              | 0.39305                | 3.1415     | 0.0726              | 0.83 | 174 $\rightarrow$ 179 |
Table S8: Computed excitation energy (eV), excitation coefficient, $\Delta r$ (Å), oscillator strength ($f$) and dipole moment ($\mu$, D) for singlet states of PPI-An and PPICN-An.

| Emitters | State | Excitation energy | Excitation coefficient | $\Delta r$ | Oscillator strength | $\mu$ | NTO Transitions |
|----------|-------|-------------------|------------------------|------------|-------------------|------|----------------|
| PPI-An   | 1     | 2.64              | 0.4595                 | 0.4388     | 0.2938            | 0.58 | 146 $\rightarrow$ 147 |
|          | 2     | 2.92              | 0.4491                 | 3.1565     | 0.8180            | 0.92 | 146 $\rightarrow$ 148 |
|          | 3     | 3.02              | 0.4393                 | 1.1199     | 0.0465            | 1.73 | 143 $\rightarrow$ 148 |
|          | 4     | 3.16              | 0.4005                 | 2.4492     | 0.1084            | 1.41 | 146 $\rightarrow$ 149 |
|          | 5     | 3.32              | 0.4595                 | 0.4388     | 0.0129            | 0.57 | 146 $\rightarrow$ 151 |
| PPICN-An | 1     | 2.64              | 0.4591                 | 0.4806     | 0.2933            | 0.61 | 150 $\rightarrow$ 151 |
|          | 2     | 2.92              | 0.4424                 | 2.9787     | 0.8523            | 0.99 | 150 $\rightarrow$ 153 |
|          | 3     | 3.03              | 0.4386                 | 1.3727     | 0.0387            | 1.84 | 147 $\rightarrow$ 153 |
|          | 4     | 3.17              | 0.4062                 | 2.9545     | 0.1336            | 2.45 | 150 $\rightarrow$ 154 |
|          | 5     | 3.29              | 0.3679                 | 2.5629     | 0.0910            | 0.64 | 150 $\rightarrow$ 152 |
Table S9: Computed excitation energy (eV), excitation coefficient, Δr (Å), oscillator strength (f) and dipole moment (μ, D) for singlet states of PPI-Py and PPICN-Py.

| Emitters   | State | Excitation energy | Excitation coefficient | Δr   | Oscillator strength | μ      | NTO Transitions |
|------------|-------|-------------------|------------------------|------|---------------------|--------|-----------------|
| PPI-Py     | 1     | 2.89              | 0.4402                 | 3.6710 | 1.7990            | 0.36   | 154 → 155       |
|            | 2     | 3.01              | 0.4152                 | 2.6923 | 0.5615            | 0.44   | 154 → 156       |
|            | 3     | 3.24              | 0.3349                 | 2.9493 | 0.1284            | 1.28   | 153 → 156       |
|            | 4     | 3.25              | 0.4160                 | 2.6497 | 0.0221            | 0.53   | 153 → 155       |
|            | 5     | 3.26              | 0.3207                 | 3.0665 | 0.0327            | 0.47   | 151 → 158       |
| PPICN-Py   | 1     | 2.89              | 0.4394                 | 4.7259 | 1.7642            | 6.17   | 158 → 160       |
|            | 2     | 3.01              | 0.4259                 | 3.6489 | 0.6147            | 5.64   | 158 → 161       |
|            | 3     | 3.23              | 0.3737                 | 4.5599 | 0.2428            | 0.99   | 158 → 162       |
|            | 4     | 3.25              | 0.4001                 | 2.6567 | 0.0232            | 0.79   | 158 → 162       |
|            | 5     | 3.25              | 0.3862                 | 2.5888 | 0.0166            | 2.25   | 158 → 162       |
Table S10: Computed RMSD of electron and hole, H index and t index for singlet states of PPI-Cz and PPICN-Cz.

| Emitters | State | RMSD (Electron) | RMSD (Hole) | H index | t index |
|----------|-------|-----------------|-------------|---------|---------|
|          |       | x    y    z    total | x    y    z    total | x    y    z    Total | x    y    z    Total |
|          |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| PPI-Cz   | S1    | 2.634 | 2.622 | 0.779 | 3.797 | 2.995 | 2.964 | 0.792 | 4.287 | 2.814 | 2.793 | 0.786 | 4.042 | -2.281 | -2.445 | -0.733 | 3.423 |
|          | S2    | 2.562 | 2.555 | 0.784 | 3.702 | 2.908 | 2.950 | 0.786 | 4.217 | 2.735 | 2.753 | 0.785 | 3.959 | -2.442 | -2.430 | -0.770 | 3.530 |
|          | S3    | 1.939 | 1.440 | 1.410 | 2.796 | 2.549 | 1.475 | 1.267 | 3.206 | 2.244 | 1.458 | 1.338 | 2.992 | -1.400 | -1.413 | -1.144 | 2.294 |
|          | S4    | 2.500 | 1.477 | 1.390 | 3.219 | 2.904 | 1.719 | 1.387 | 3.649 | 2.702 | 1.598 | 1.389 | 3.433 | -2.339 | -1.506 | -1.306 | 3.073 |
|          | S5    | 4.001 | 3.123 | 0.871 | 5.150 | 3.655 | 2.720 | 0.822 | 4.630 | 3.828 | 2.921 | 0.847 | 4.889 | -2.661 | -2.851 | -0.674 | 3.957 |
| PPICN-Cz | S1    | 0.944 | 0.955 | 0.769 | 1.548 | 2.072 | 1.277 | 0.753 | 2.547 | 1.508 | 1.116 | 0.761 | 2.025 | 0.114  | -0.331 | -0.270 | 0.442 |
|          | S2    | 1.226 | 1.021 | 0.776 | 1.774 | 1.102 | 1.255 | 0.990 | 1.941 | 1.164 | 1.138 | 0.883 | 1.852 | -0.441 | -0.424 | -0.674 | 0.910 |
|          | S3    | 0.898 | 0.947 | 0.748 | 1.505 | 1.800 | 1.378 | 0.720 | 2.378 | 1.349 | 1.162 | 0.734 | 1.926 | 0.097  | -0.119 | -0.334 | 0.368 |
|          | S4    | 1.387 | 2.578 | 0.807 | 3.036 | 1.866 | 2.539 | 0.779 | 3.246 | 1.626 | 2.558 | 0.793 | 3.134 | -0.879 | -1.633 | -0.455 | 1.910 |
|          | S5    | 2.448 | 2.959 | 0.933 | 3.952 | 1.781 | 2.822 | 0.784 | 3.428 | 2.114 | 2.891 | 0.859 | 3.683 | -1.985 | -2.277 | -0.775 | 3.118 |
Table S11: Computed RMSD of electron and hole, H index and t index for singlet states of PPI-An and PPICN-An

| Emitters | State | RMSD (Electron) | RMSD (Hole) | H index | t index |
|----------|-------|-----------------|-------------|---------|---------|
|          |       | x    | y    | z    | total | x    | y    | z    | total | x    | y    | z    | Total | x    | y    | z    | Total |
| PPI-An   | S1    | 2.032| 3.997| 0.875| 4.569 | 1.530| 3.210| 0.843| 3.655| 1.781| 3.604| 0.859| 4.111| -1.640| -3.248| -0.776| 3.720 |
|          | S2    | 2.165| 4.244| 0.924| 4.853 | 1.556| 3.256| 3.256| 3.707| 1.861| 3.750| 0.884| 4.279| -1.234| -3.603| -0.857| 3.903 |
|          | S3    | 1.727| 3.758| 0.901| 4.233 | 1.530| 3.210| 0.843| 3.655| 1.629| 3.484| 0.872| 3.944| -0.685| -2.595| -0.733| 2.782 |
|          | S4    | 2.969| 2.952| 0.834| 4.269 | 1.729| 3.388| 0.846| 3.897| 2.349| 3.170| 0.840| 4.034| -1.341| -2.503| -0.706| 2.926 |
|          | S5    | 3.142| 3.934| 0.875| 5.111 | 2.321| 4.155| 0.843| 4.834| 2.732| 4.045| 0.859| 4.956| -2.581| -3.612| -0.797| 4.510 |
| PPICN-An | S1    | 2.127| 3.954| 0.990| 4.597 | 1.515| 3.193| 0.923| 3.653| 1.821| 3.574| 0.957| 4.123| -1.593| -3.243| -0.859| 3.714 |
|          | S2    | 2.054| 4.233| 1.039| 4.819 | 1.515| 3.193| 0.923| 3.653| 1.785| 3.713| 0.981| 4.235| -1.100| -3.555| -0.920| 3.833 |
|          | S3    | 1.915| 3.700| 1.020| 4.289 | 1.515| 3.193| 0.923| 3.653| 1.715| 3.446| 0.972| 3.970| -0.912| -2.326| -0.809| 2.626 |
|          | S4    | 3.500| 2.669| 1.017| 4.518 | 1.795| 3.227| 0.934| 3.809| 2.647| 2.948| 0.976| 4.081| -0.618| -2.760| -0.880| 2.962 |
|          | S5    | 3.313| 3.865| 0.968| 5.182 | 2.248| 3.920| 0.906| 4.609| 2.781| 3.893| 0.937| 4.875| -2.424| -3.510| -0.836| 4.347 |
Table S12: Computed RMSD of electron and hole, H index and t index for singlet states of PPI-Py and PPICN-Py.

| Emitters | State | RMSD (Electron) | RMSD (Hole) | H index | t index |
|----------|-------|-----------------|-------------|---------|---------|
|          |       | x   | y   | z   | total | x   | y   | z   | total | x   | y   | z   | total |
| PPI-Py   | S1    | 4.775 | 4.520 | 0.705 | 6.613 | 4.518 | 4.231 | 0.713 | 6.231 | 4.647 | 4.376 | 0.709 | 6.422 | -4.437 | -4.274 | -0.686 | 6.199 |
|          | S2    | 4.903 | 3.472 | 0.699 | 6.049 | 4.734 | 3.366 | 0.713 | 5.852 | 4.819 | 3.419 | 0.706 | 5.950 | -4.534 | -3.319 | -0.678 | 5.659 |
|          | S3    | 4.324 | 4.778 | 0.783 | 6.491 | 4.290 | 4.347 | 0.709 | 6.148 | 4.307 | 4.562 | 0.746 | 6.318 | -3.206 | -4.558 | -0.710 | 5.618 |
|          | S4    | 3.540 | 2.414 | 0.678 | 4.338 | 3.858 | 2.518 | 0.706 | 4.661 | 3.699 | 2.466 | 0.692 | 4.499 | -3.339 | -2.406 | -0.677 | 4.171 |
|          | S5    | 3.733 | 4.330 | 0.730 | 5.763 | 3.435 | 3.446 | 0.594 | 4.902 | 3.584 | 3.888 | 0.662 | 5.329 | -3.384 | -3.505 | -0.598 | 4.908 |
| PPICN-Py | S1    | 4.749 | 4.504 | 0.723 | 6.585 | 4.638 | 4.267 | 0.725 | 6.344 | 4.694 | 4.386 | 0.724 | 6.465 | -4.303 | -4.275 | -0.718 | 6.108 |
|          | S2    | 4.872 | 3.340 | 0.714 | 5.950 | 4.608 | 3.297 | 0.732 | 5.713 | 4.740 | 3.318 | 0.723 | 5.831 | -4.693 | -2.832 | -0.704 | 5.526 |
|          | S3    | 2.905 | 4.882 | 0.797 | 5.737 | 3.284 | 4.080 | 0.732 | 5.288 | 3.095 | 4.481 | 0.765 | 5.499 | -0.766 | -2.452 | -0.764 | 2.680 |
|          | S4    | 3.904 | 2.503 | 0.703 | 4.691 | 3.941 | 2.484 | 0.735 | 4.716 | 3.923 | 2.493 | 0.719 | 4.703 | -3.808 | -2.432 | -0.703 | 4.572 |
|          | S5    | 3.349 | 3.982 | 0.730 | 5.254 | 3.534 | 3.867 | 0.722 | 5.288 | 3.441 | 3.924 | 0.726 | 5.270 | -2.878 | -3.741 | -0.705 | 4.772 |
Table S13. Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipolemoment (\(\mu\)) for singlet states of PPI-Cz and PPICN-Cz.

| Emitters | State | Hole integral | Electron integral | Integral of transition density | Integral overlap of h\(^+\) - e\(^-\) (S) | Centroid of hole (Å) | Centroid of electron (Å) | D (Å) | \(\mu\) (a.u) |
|----------|-------|---------------|-------------------|-------------------------------|----------------------------------------|----------------------|------------------------|-------|----------|
|          |       |               |                   |                               | x   | y   | z | x | y | z |                   |       |           |
| PPI-Cz   | S1    | 0.7525        | 0.5694            | -0.0008                       | 0.4105 | -0.8571 | -0.2758 | 0.0775 | -1.3902 | -0.6238 | 0.0244   | 0.6388 | 0.7980   |
|          | S2    | 0.7113        | 0.5452            | -0.0023                       | 0.2521 | -1.1280 | -0.5652 | 0.2499 | -1.4207 | -0.2422 | 0.2651   | 0.4361 | 0.5178   |
|          | S3    | 0.8311        | 0.6360            | -0.0148                       | 0.5008 | -5.7770 | 1.1974  | 0.1429 | -6.6209 | 1.1526  | 0.3377   | 0.8672 | 1.2022   |
|          | S4    | 0.8091        | 0.5734            | -0.0005                       | 0.3910 | -5.8132 | 1.1163  | 0.1957 | -6.1761 | 1.2081  | 0.2783   | 0.3833 | 0.5008   |
|          | S5    | 0.7259        | 0.5570            | -0.0081                       | 0.3385 | -1.2190 | -1.1530 | 0.2952 | -2.3864 | -1.0827 | 0.1224   | 1.1822 | 1.4332   |
| PPICN-Cz | S1    | 0.9260        | 0.8306            | 0.0295                        | 0.1563 | 5.0523  | 3.5413  | 0.4267 | 6.6742  | 4.3260  | -0.0643  | 1.8674 | 3.0997   |
|          | S2    | 0.8783        | 0.8198            | 0.0064                        | 0.2677 | 7.1784  | -2.3760 | 0.0266 | 7.9012  | -1.6621 | 0.2359   | 1.0371 | 1.6642   |
|          | S3    | 0.8306        | 0.7831            | -0.0016                       | 0.3083 | 6.5779  | -2.6614 | -0.1321 | 8.0242  | -1.6179 | 0.2682   | 1.8278 | 2.7870   |
|          | S4    | 0.8518        | 0.7497            | -0.0084                       | 0.3522 | 5.8628  | 2.4269  | 0.2531 | 6.6102  | 3.3523  | -0.0852  | 1.2367 | 1.8715   |
|          | S5    | 0.7294        | 0.6647            | 0.0060                        | 0.3281 | 6.4611  | -1.3069 | -0.0131 | 6.5907  | -0.6933 | -0.0965  | 0.6327 | 0.8335   |
Table S14. Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipole moment (µ) for singlet states of PPI-An and PPICN-An.

| Emitters | State | Hole integral | Electron integral | Integral of transition density | Integral overlap of h⁺ - e⁻ (S) | Centroid of hole (Å) | Centroid of electron (Å) | D (Å) | µ (a.u) |
|----------|-------|---------------|------------------|-----------------------------|-------------------------------|----------------------|------------------------|-------|--------|
|          |       |               |                  |                             |                               | x        | y        | z      |        |
|          |       |               |                  |                             |                               | x        | y        | z      |        |
|          |       |               |                  |                             |                               |          |          |        |        |
| PPI-An   | S1    | 0.8031        | 0.7620           | -0.0024                    | 0.39176                       | 3.9365   | 0.6275   | -0.0714| 3.7956 | 0.2712 | -0.1546| 0.3920 | 0.5798 |
|          | S2    | 0.7873        | 0.7222           | -0.0241                    | 0.25060                       | 3.9160   | 0.6450   | -0.0714| 4.5431 | 0.7926 | -0.0440| 0.6447 | 0.9197 |
|          | S3    | 0.7678        | 0.6368           | 0.0076                     | 0.21810                       | 3.9365   | 0.6275   | -0.0714| 4.8798 | -0.2616| -0.2102| 1.3037 | 1.7303 |
|          | S4    | 0.7089        | 0.5185           | 0.0396                     | 0.25036                       | 3.8037   | 0.4502   | -0.1070| 2.7958 | 1.1166 | 0.0276 | 1.2157 | 1.4101 |
|          | S5    | 0.7014        | 0.6155           | -0.0102                    | 0.39870                       | 2.6678   | 1.4608   | -0.0479| 2.8185 | 1.0277 | -0.1095| 0.4626 | 0.5757 |
| PPICN-An | S1    | 0.8014        | 0.7611           | -0.0026                    | 0.3868                        | 4.1224   | 0.4474   | -0.0514| 3.8940 | 0.1167 | -0.1492| 0.4135 | 0.6105 |
|          | S2    | 0.7723        | 0.7133           | -0.0279                    | 0.2350                        | 4.1224   | 0.4474   | -0.0514| 4.8067 | 0.6056 | 0.0094 | 0.7050 | 0.9897 |
|          | S3    | 0.7656        | 0.6354           | 0.0064                     | 0.2144                        | 4.1224   | 0.4474   | -0.0514| 4.9256 | 0.6732 | -0.2145| 1.3883 | 1.8379 |
|          | S4    | 0.7149        | 0.5553           | -0.0300                    | 0.2217                        | 4.1224   | 0.3206   | -0.0781| 1.9269 | 0.5084 | 0.0181 | 2.0400 | 2.4485 |
|          | S5    | 0.6781        | 0.5887           | 0.0200                     | 0.3909                        | 3.2074   | 1.7136   | 0.0217 | 2.8512 | 1.3312 | -0.0793| 0.5323 | 0.6372 |
Table S15. Computed hole and electron overlap (S), distance between centroids of hole and electron (D, Å) and dipolemoment (µ) for singlet states of PPI-Py and PPICN-Py.

| Emitters | State | Hole integral | Electron integral | Integral of transition density | Integral overlap of $h^+\cdot e^-$ (S) | Centroid of hole (Å) | Centroid of electron (Å) | D (Å) | µ (a.u) |
|----------|-------|----------------|-------------------|-----------------------------|---------------------------------|---------------------|----------------------|-------|--------|
|          |       |                |                   |                             | $x$    | $y$     | $z$   | $x$    | $y$     | $z$   |       |
| PPI-Py   | S1    | 0.8935         | 0.7392            | 0.0039                     | 0.5904 | 0.7264  | 2.8450| -0.0421| 0.5171  | 2.7430| -0.0190| 0.2340| 0.3610|
|          | S2    | 0.8445         | 0.6970            | -0.0017                    | 0.5686 | 4.7985  | 0.2374| -0.0226| 5.0830  | 0.1371| 0.0054 | 0.3030| 0.4413|
|          | S3    | 0.6914         | 0.5349            | -0.0068                    | 0.3873 | 0.3021  | 2.6139| -0.0537| -0.7986 | 2.6096| -0.0179| 1.1013| 1.2761|
|          | S4    | 0.8776         | 0.6515            | -0.0010                    | 0.5468 | 6.6156  | -0.6428| 0.0163 | 6.9755  | -0.5826| 0.0310 | 0.3651| 0.5276|
|          | S5    | 0.6109         | 0.5235            | -0.0042                    | 0.3025 | -1.0973 | 3.3245| -0.0909| -1.2974 | 3.7081| -0.0267| 0.4373| 0.4688|
| PPICN-Py | S1    | 0.8938         | 0.7370            | 0.0046                     | 0.59417| 1.2128  | 2.8846| -0.0826| 0.8223  | 2.7733| -0.0762| 0.4060| 0.6257|
|          | S2    | 0.8682         | 0.7152            | 0.0008                     | 0.57016| 5.2887  | 0.0342| 0.0113 | 5.3361  | -0.4518| 0.0300 | 0.4888| 0.7313|
|          | S3    | 0.7632         | 0.6168            | -0.0131                    | 0.30408| 0.1630  | 0.8140| -0.2433| -2.1654 | -1.2152| -0.2444| 3.0886| 4.0279|
|          | S4    | 0.8454         | 0.6277            | 0.0001                     | 0.54633| 6.6886  | -0.7453| 0.0730 | 6.8036  | -0.6840| 0.0887 | 0.1313| 0.1827|
|          | S5    | 0.8166         | 0.6084            | 0.0023                     | 0.5132 | -0.6419 | 4.6308| -0.0900| -1.20586| 4.8139| -0.0693| 0.5932| 0.7988|