Modulation of Luminescence Properties of Circularly Polarized Thermally Activated Delayed Fluorescence Molecules with Axial Chirality by Donor Engineering

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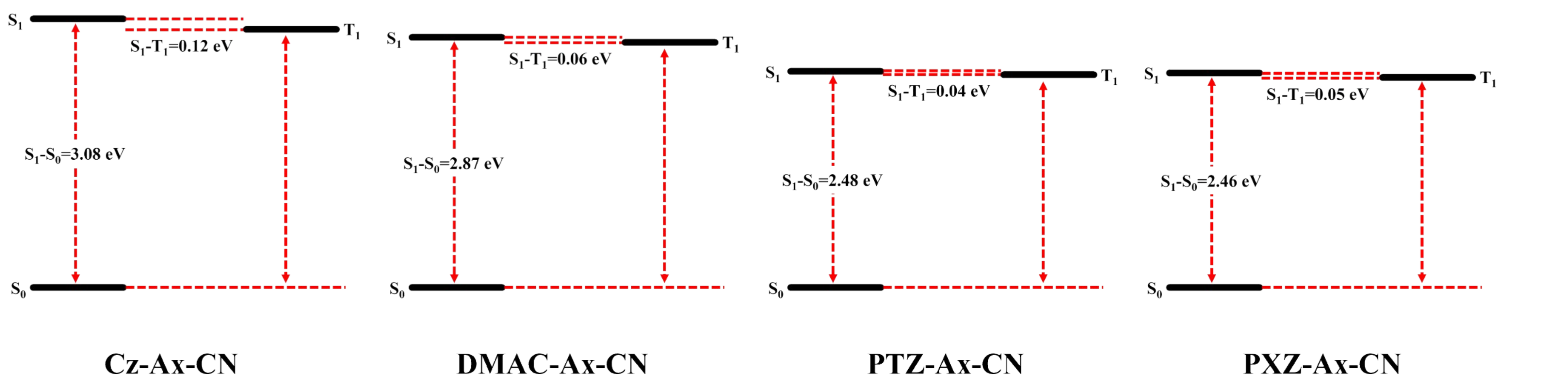

Figure S1. The energy levels of molecules of Cz-Ax-CN, DMAC-Ax-CN, PTZ-Ax-CN and PXZ-Ax-CN in toluene.

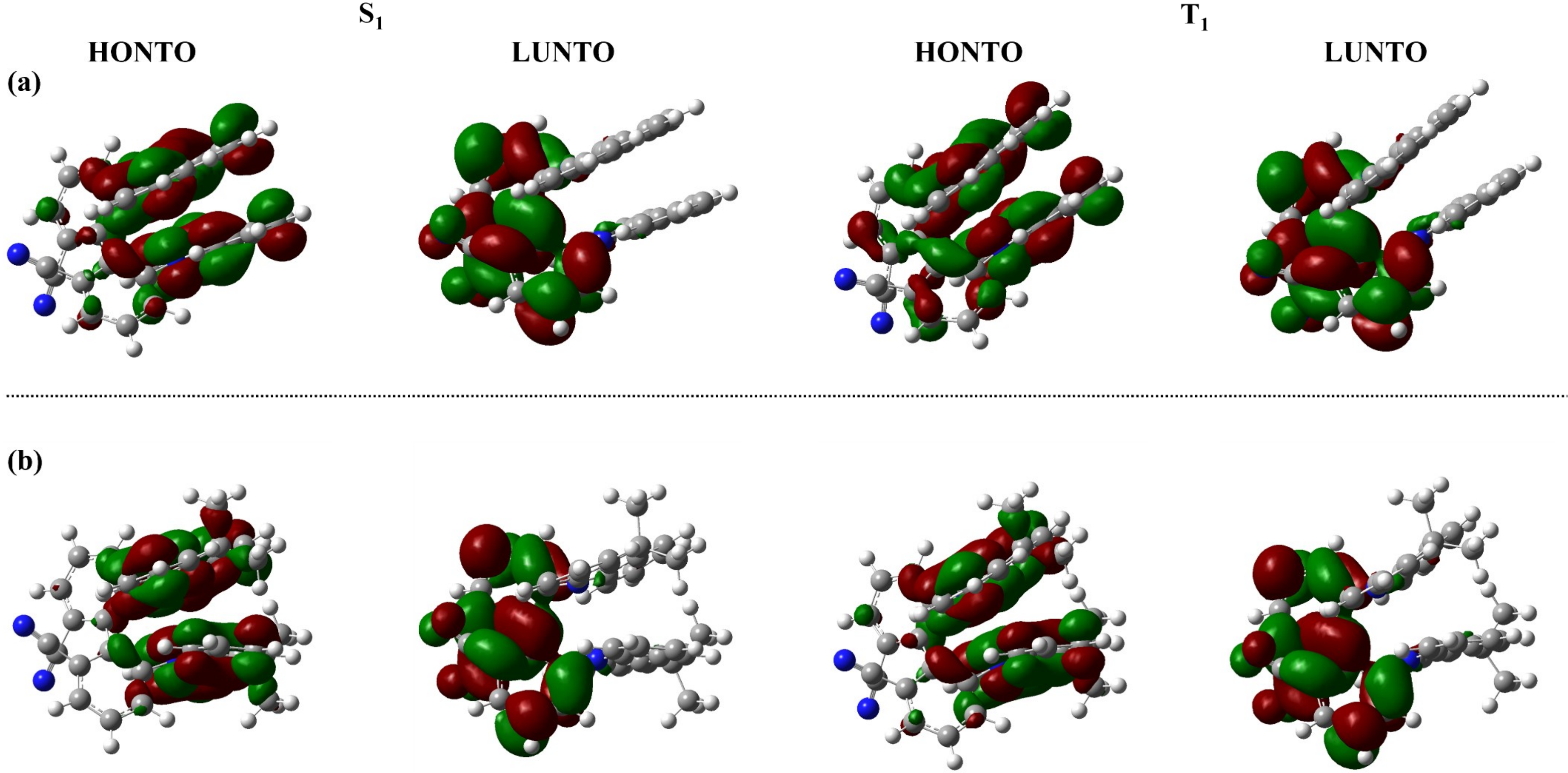

Figure S2. Natural transition orbitals (NTOs) of the S_1 and T_1 states for (a) Cz-Ax-CN and (b) DMAC-Ax-CN in toluene, respectively.

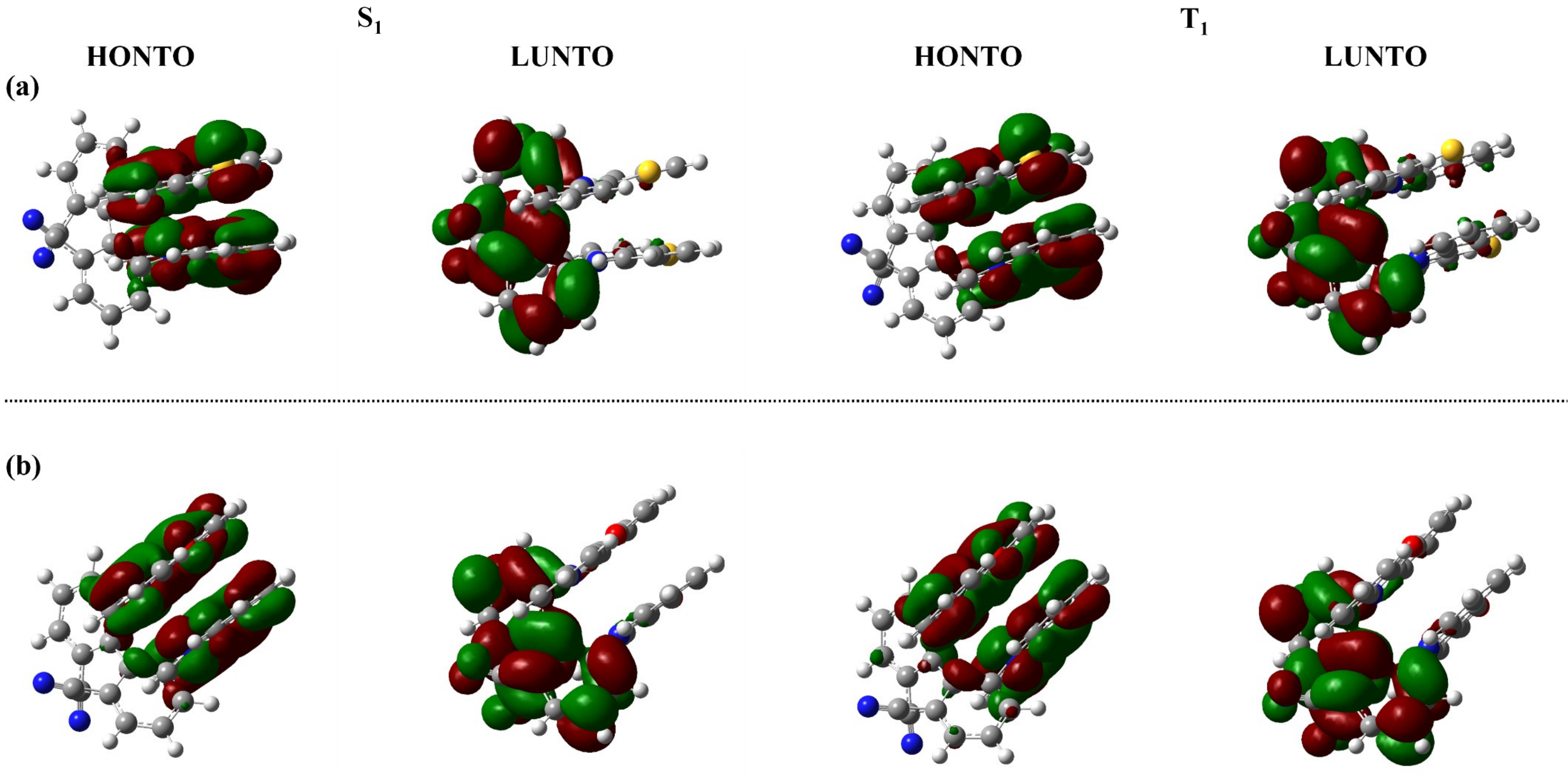

Figure S3. Natural transition orbitals (NTOs) of the S_1 and T_1 states for (a) PTZ-Ax-CN and (b) PXZ-Ax-CN in toluene, respectively.

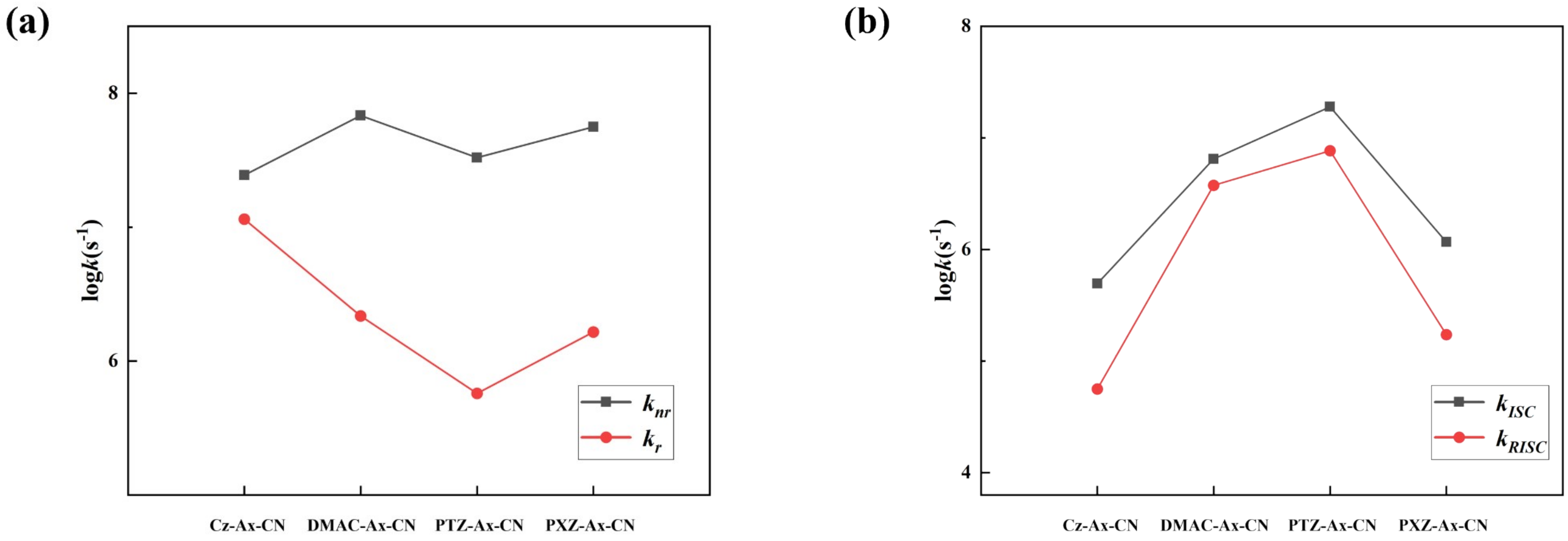

Figure S4. Rates constants of Radiative and Non-Radiative from S_1 to S_0 as well as the ISC and RISC rates between S_1 and T_1 for all studied molecules in toluene.

Table S1. The overlap and orbital energies of HOMO and LUMO are listed, the ε_{gap} is the energy gap between the HOMO and LUMO.

	HOMO (eV)	LUMO (eV)	ε_{gap} (eV)	Overlap
Cz-Ax-CN	-6.01	-1.25	4.75	28.31%
DMAC-Ax-CN	-5.70	-1.18	4.52	26.43%
PTZ-Ax-CN	-5.48	-1.31	4.18	25.58%
PXZ-Ax-CN	-5.46	-1.24	4.23	25.60%

Table S2. The data of absorption asymmetry factor (g_{abs}) for Cz-Ax-CN, DMAC-Ax-CN, PTZ-Ax-CN and PXZ-Ax-CN in toluene.

	$\lvert\mu\rvert$ ($\times 10^{-18}$ esu·cm)	$\lvert m\rvert$ ($\times 10^{-20}$ erg·G^{-1})	cos θ	g_{abs} ($\times 10^{-2}$)
Cz-Ax-CN	1.450	0.532	-1	-1.47
DMAC-Ax-CN	1.108	0.190	-1	-6.87
PTZ-Ax-CN	0.703	0.392	-1	-2.23
PXZ-Ax-CN	0.980	0.296	-1	-1.21