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Electronic Supplementary Information

A quantitative description of photoluminescence efficiency of a carbazole-based thermally activated delayed fluorescence emitter

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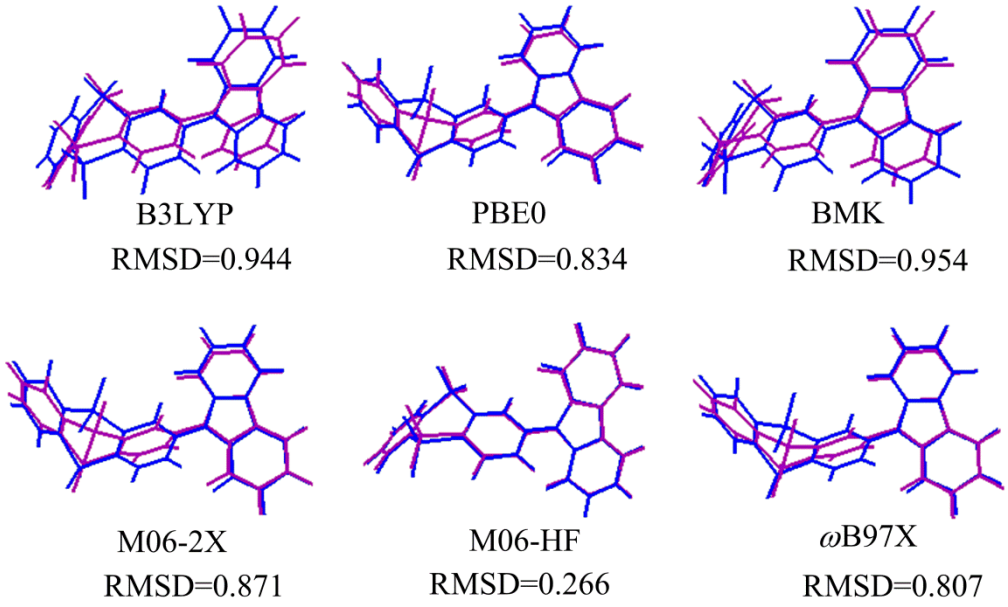

Fig. S1 Geometry comparisons between S_0 (blue) and S_1 (purple) calculated using different density functionals for **CZ-TTR**.

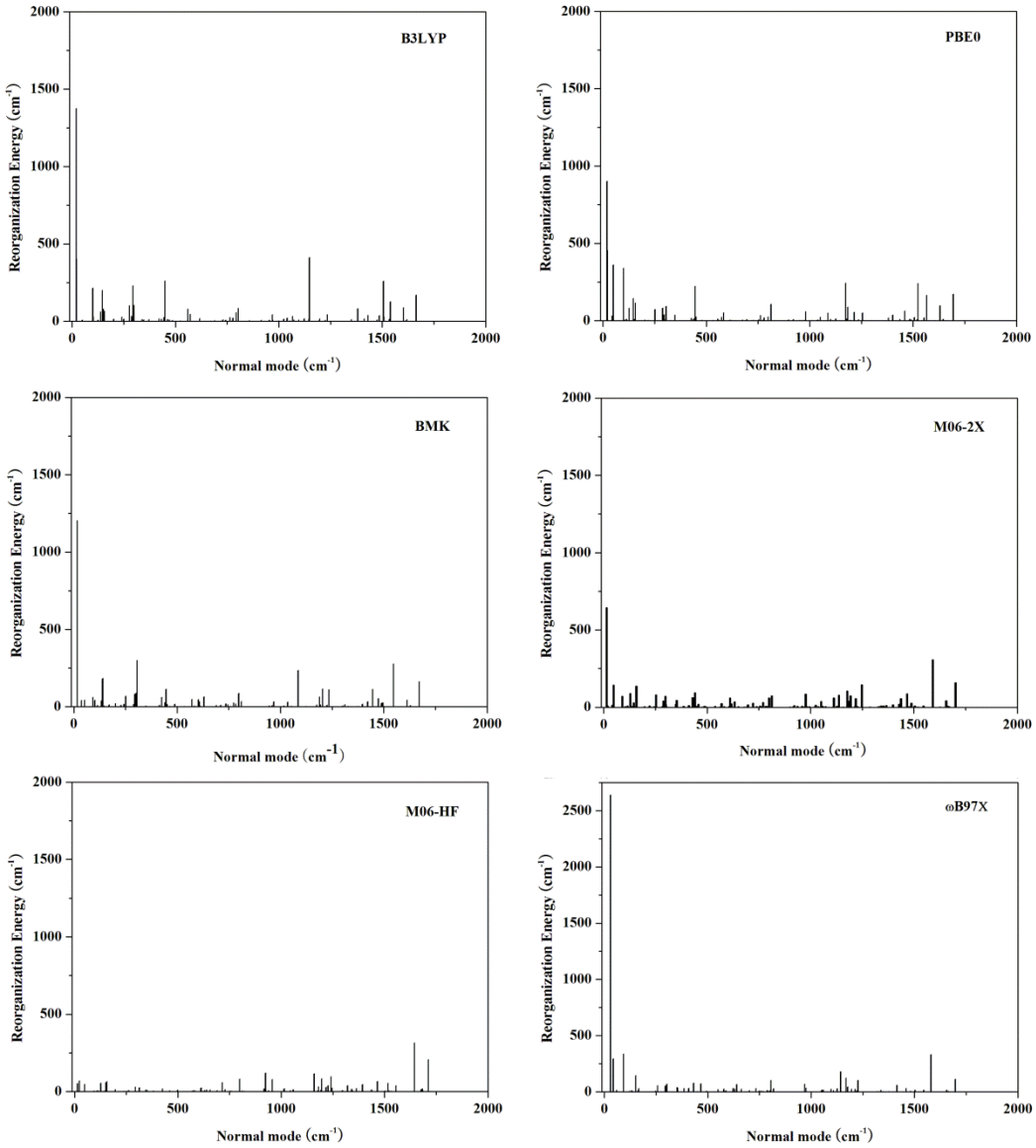

Fig. S2 Reorganization energy of each normal vibration mode calculated using different density functionals for **CZ-TTR**.

Table S1 Reorganization energies (meV) from bond length, bond angle, and dihedral angle in the gas phase

	Bond length	Bond angle	Dihedral angle	Total
λ	210.7	48.3	39.4	298.4

Table S2 Excited-state decay rate constants obtained by the M06-HF/B3LYP hybrid calculations at different temperatures (in unit of s^{-1})

Temperature/K	k_r^S	k_{nr}^S	k_{ISC}	k_{RISC}	k_r^T	k_{nr}^T
77	3.59×10^5	7.13×10^4	2.86×10^4	2.25×10^3	1.00	1.90×10^4
100	3.47×10^5	7.29×10^4	9.24×10^4	1.11×10^4	0.98	2.20×10^4
150	3.40×10^5	7.74×10^4	3.86×10^5	9.15×10^4	0.96	3.17×10^4
200	3.42×10^5	8.36×10^4	8.15×10^5	2.90×10^5	0.93	4.78×10^4
250	3.45×10^5	9.23×10^4	1.29×10^6	5.87×10^5	0.90	7.36×10^4
300	3.47×10^5	1.04×10^5	1.75×10^6	9.41×10^5	0.87	1.13×10^5