Supporting Information

Theoretical Study on the Light-emitting Mechanism of Circularly Polarized Luminescence Molecules with both Thermally Activated Delayed Fluorescence and Aggregation Induced Emission

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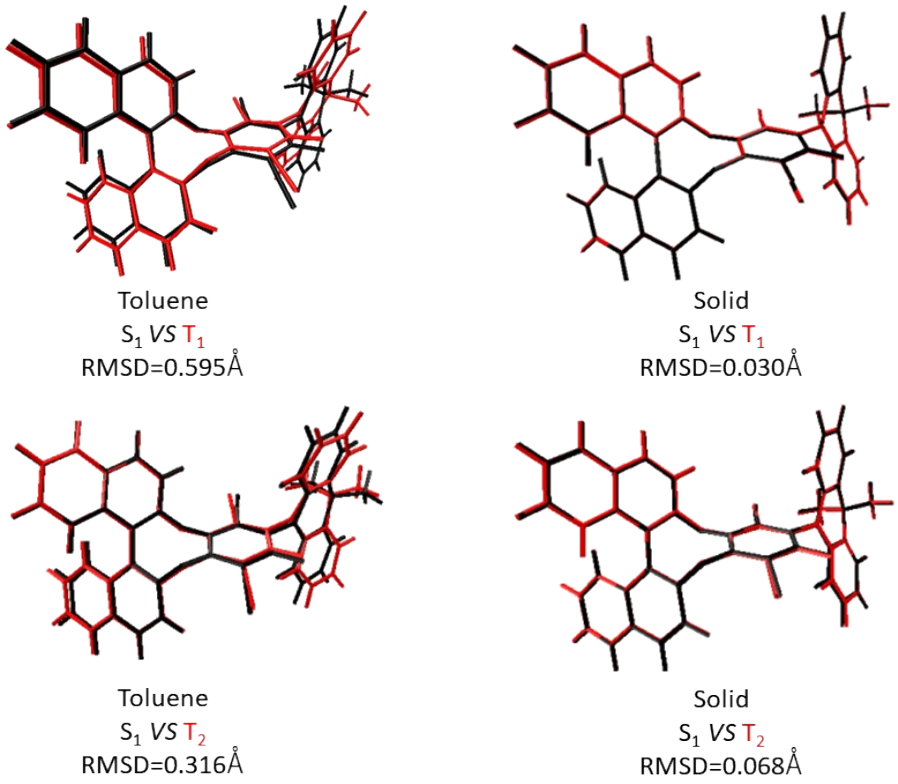

Fig. S1 Visible geometry changes between S_1 (black) and two triplet excited states (red) in toluene and solid phase for S-BN-AF respectively.

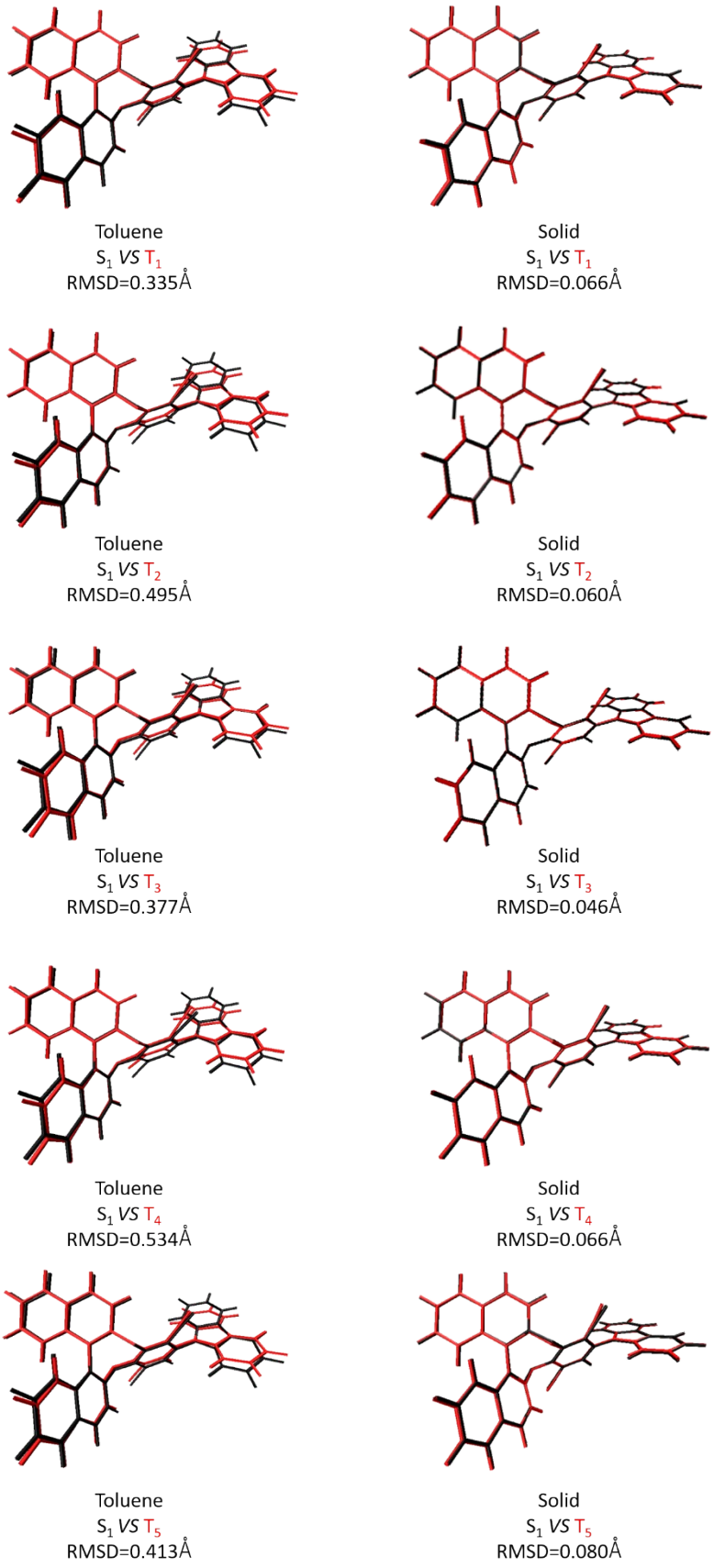

Fig. S2 Visible geometry changes between S_1 (black) and five triplet excited states

(red) in toluene and solid phase for R-BN-CF respectively.

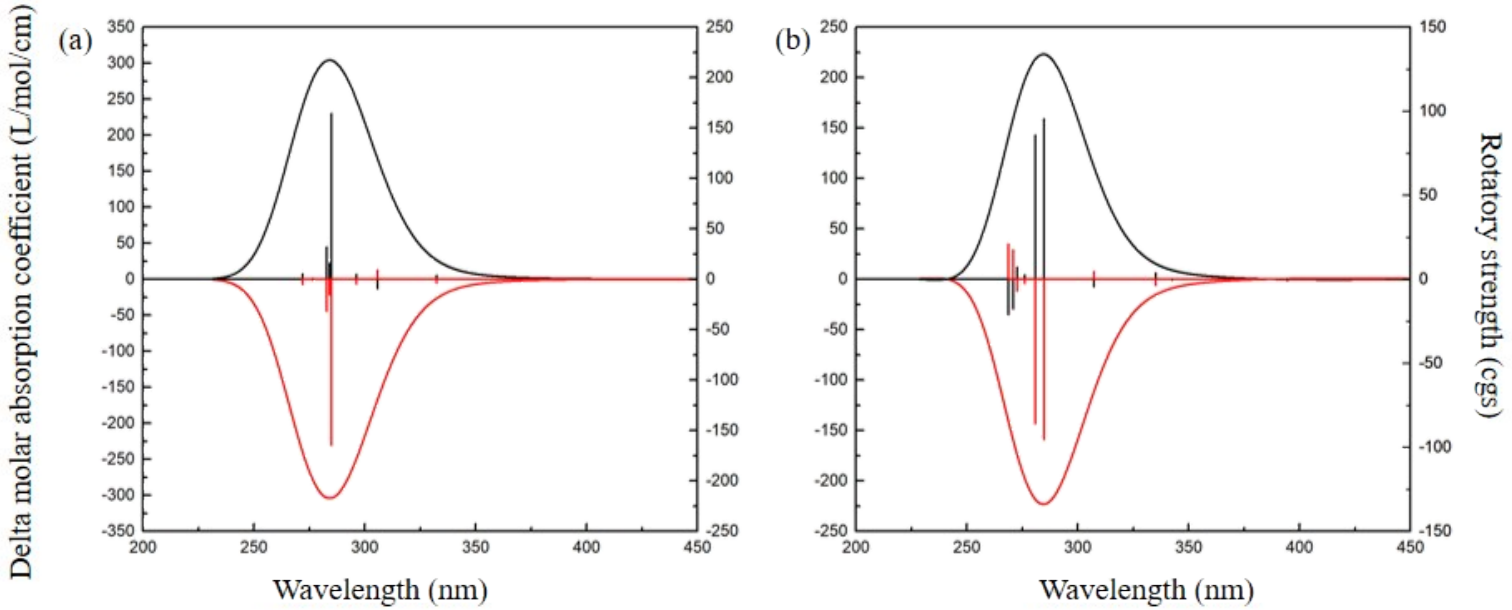

Fig. S3 ECD spectra for R-BN-AF (black) and S-BN-AF (red) (a) as well as R-BN-CF (black) and S-BN-CF (red) (b) in toluene. The rotatory strength is also illustrated.

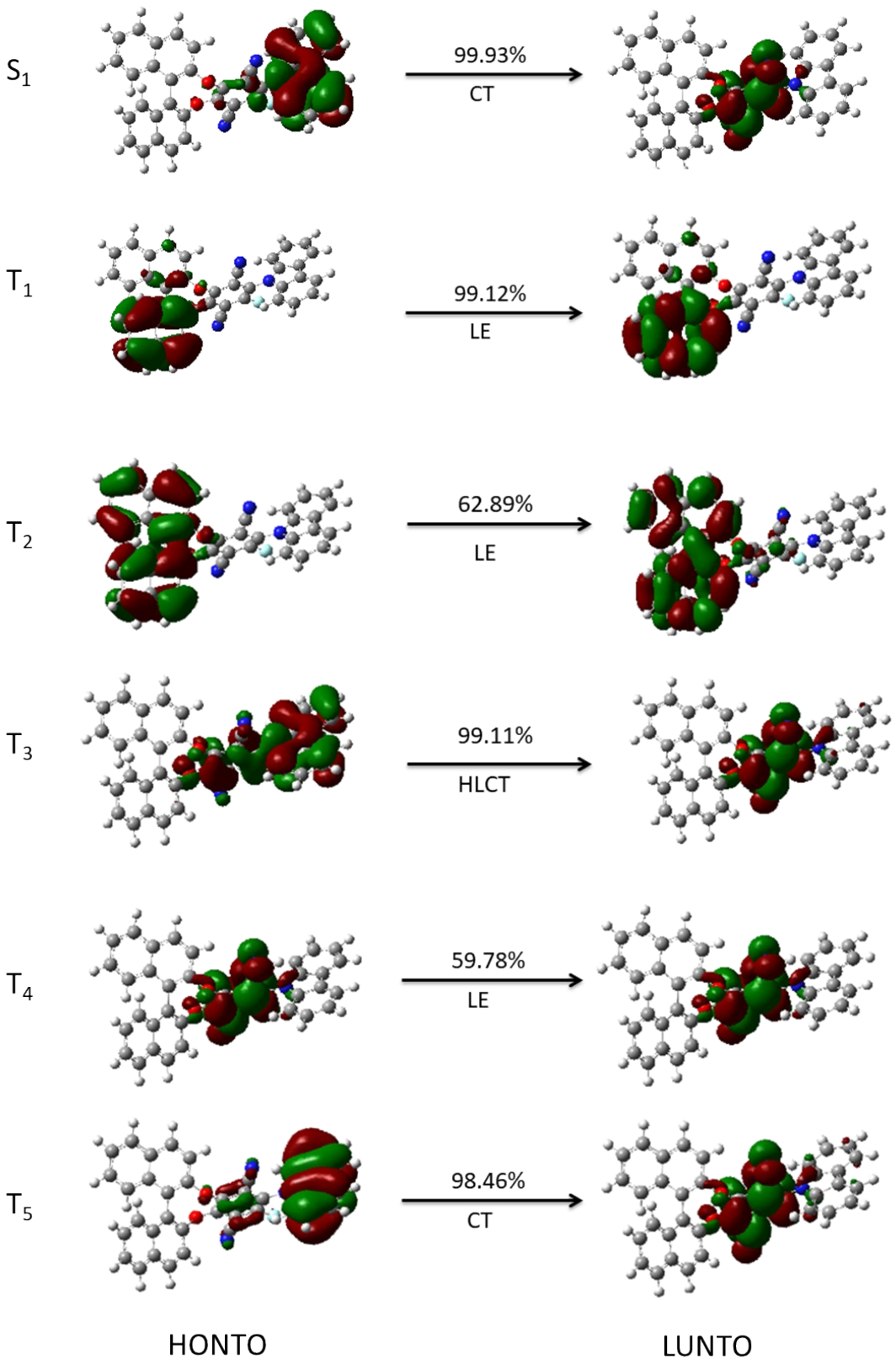

Fig. S4 Transition characteristics for S_1, T_1, T_2, T_3, T_4 and T_5 sates of R-BN-CF in toluene. The value above every arrow represents the ratio of depicted NTOs in the

corresponding transition.

Table S1. The local excitation (LE) ratio for each singlet and triplet excited state for S-BN-AF respectively.

	S_1	T_1	T2
toluene	16.31%	40.70%	19.32%
solid	20.56%	39.06%	38.90%

Table S2. The local excitation (LE) ratio for each singlet and triplet excited state for R-BN-CF respectively.

	S_1	T_1	T_2	T_3	T_4	T_5
toluene	21.33%	90.53%	86.06%	59.80%	80.98%	32.98%
solid	34.69%	90.23%	85.78%	65.16%	82.27%	74.55%