Electronic Supporting Information

Intramolecular charge transfer in aminobenzonitriles and tetrauoro counterparts: fluorescence explained by competition between low lying excited states and radiationless deactivation.
Part II: Influence of substitution on luminescence patterns

Mireia Segado, Yannick Mercier, Isabel Gómez, Mar Reguero
Figure 1.- Schematic representation of the orbitals included in the CAS(12,11). $R_1 = \text{H,CH}_3$; $R_2 = \text{H,F}$. 

Figure S2.- Geometries and electronic structures (in red) of the ground state, LE, TICT, and RICT minima in DMABN-4F. All bond lengths are in Å. Values of the second-order exchange density matrix (in italic blue) and the one-electron density matrix (in black) for the same structures.
Figure S3. Geometry of the lowest energy excited state minima of ABN, DMABN, ABN-4F and DMBN-4F optimized at the CASSCF(12,11)/6-31G* level. Bond distances in Å.
Figure S4.- Geometry of the $S_2/S_1$ ICT(Q)/ICT(CN) conical intersection for ABN-4F optimized at CASSCF(12,11)/6-31G(d) level.

Figure S5.- MS-CASPT2 profiles of the LE and ICT states of ABN-4F along the LIIC path from LE to TICT minima.

Figure S6.- Geometry of the ICT(Q)/LE ($S_2/S_1$) conical intersection and vectors of the branching space for DMABN-4F: a) derivative coupling; b) gradient difference.
Figure S7.- MS-CASPT2 profiles of the LE and ICT states of DMABN-4F along the LIIC path from FC to the LE minimum

Figure S8.- Geometries of the $S_1/S_0$ conical intersections located for ABN-4F at CASSCF level.
Figure S9.- MS-CASPT2 profiles of the LE and ground state potential energy surfaces of ABN-4F along LIIC path from the LE minima to different S1/S0 conical intersections: a) LE/GS CI-1; b) LE/GS CI-2; c) LE/GS CI-3.

Figure S10.- Geometries of the S1/S0 conical intersections located for DMABN and DMABN-4F at CASSCF level: a) LE/GS CI in DMABN; b) LE/GS CI in DMABN-4F; c) CT/GS CI in DMABN; d) TS to CT/GS CI in DMABN.