Donor-Pyrene-Acceptor Distance-Dependent Intramolecular Charge-Transfer Process: A State-Specific Solvation Preferred to the Linear-Response Approach

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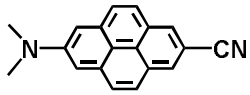
Table S1: B3LYP/SS-CPCM and LR-CPCM results for the $DANP_0$ molecule in n-hex, THF, and ACN solvents.

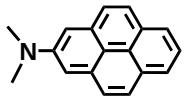
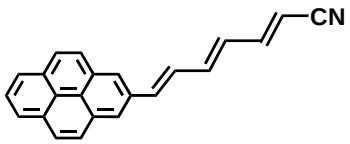
ICT molecule	**Solvent**	**λ_{abs} (nm)** ($S_0 \rightarrow S_1$)	**f_{osc}**	**λ_{em} (nm)** ($S_1 \rightarrow S_0$)	**$\Delta\nu = \nu_a - \nu_f$ (cm^{-1})**
 **$DANP_0$**	n-hex	438 (410)	0.036	494 (451)	2588 (2217)
	THF	461 (418)	0.035	609 (464)	5272 (2372)
	ACN	464 (421)	0.033	663 (469)	6469 (2431)

The values within parenthesis represent the B3LYP/LR-CPCM results

Table S2: The dipole moments of different ground- and excited-state structures in different solvents.

Solvent	Molecules	Step1	Step3	Step4	Step6	Step7
vacuo	$DANP_0$	8.68	8.68	9.05	-	-
	$DANP_1$	9.30	9.30	9.79		
	$DANP_2$	9.77	9.77	10.38		
	$DANP_3$	10.18	10.18	12.04		
n-hex	$DANP_0$	9.63	15.12	10.12	15.59	10.11
	$DANP_1$	10.16	15.39	10.80	15.64	10.79
	$DANP_2$	10.61	16.04	11.44	16.12	11.43
	$DANP_3$	11.05	21.61	13.75	25.18	13.74
DOX	$DANP_0$	9.81	15.49	10.33	16.14	10.42
	$DANP_1$	10.33	15.72	10.99	16.13	11.07
	$DANP_2$	10.77	16.36	11.66	16.62	11.73
	$DANP_3$	11.20	25.09	14.11	26.33	14.30
$CHCl_3$	$DANP_0$	10.46	16.41	11.06	18.12	11.77
	$DANP_1$	10.88	16.53	11.65	17.90	12.26
	$DANP_2$	11.30	17.10	14.34	29.05	15.90
	$DANP_3$	11.71	27.63	15.44	30.57	17.03
THF	$DANP_0$	10.73	16.68	11.34	18.88	12.38
	$DANP_1$	11.07	16.70	11.89	18.60	12.80
	$DANP_2$	11.48	17.23	14.80	30.35	17.13
	$DANP_3$	11.88	26.29	15.97	32.19	18.39
ACN	$DANP_0$	11.07	16.96	11.75	20.04	13.36
	$DANP_1$	11.34	16.93	12.24	19.71	13.67
	$DANP_2$	11.73	17.40	15.53	32.17	19.11
	$DANP_3$	12.14	23.38	16.82	34.56	20.64
BuOH	$DANP_0$	10.98	16.99	11.61	19.71	13.00
	$DANP_1$	11.27	16.96	12.14	19.38	13.35
	$DANP_2$	11.67	17.45	15.31	31.66	18.37
	$DANP_3$	12.08	26.49	16.57	33.89	19.80
EtOH	$DANP_0$	11.03	16.96	11.68	19.90	13.22
	$DANP_1$	11.31	16.93	12.19	19.57	13.55
	$DANP_2$	11.71	17.41	15.44	31.96	18.82
	$DANP_3$	12.11	24.37	16.72	34.28	20.31
MeOH	$DANP_0$	11.06	16.91	11.72	20.01	13.37
	$DANP_1$	11.33	16.88	12.23	19.68	13.68
	$DANP_2$	11.73	17.35	15.51	32.12	19.13
	$DANP_3$	12.14	22.61	16.80	34.50	20.66
H_2O	$DANP_0$	11.12	17.0	11.81	20.22	13.52
	$DANP_1$	11.38	16.96	12.29	19.89	13.81
	$DANP_2$	11.77	17.42	15.64	32.43	19.43
	$DANP_3$	12.18	22.89	16.96	34.91	21.01

Table S3: Calculated spectroscopic parameters for supporting molecules in n-hex and ACN solvents.

ICT molecules	Solvent	λ_{abs} (nm) ($S_0 \rightarrow S_1$)	f_{osc}	λ_{em} (nm) ($S_1 \rightarrow S_0$)	$\Delta\nu=\nu_a-\nu_f$ (cm^{-1})
 **DAP**	n-hex	355	0.065	385	2195
	ACN	365	0.063	439	4618
 **NP_3**	n-hex	344	2.258	415	4973
	ACN	348	2.289	440	6008

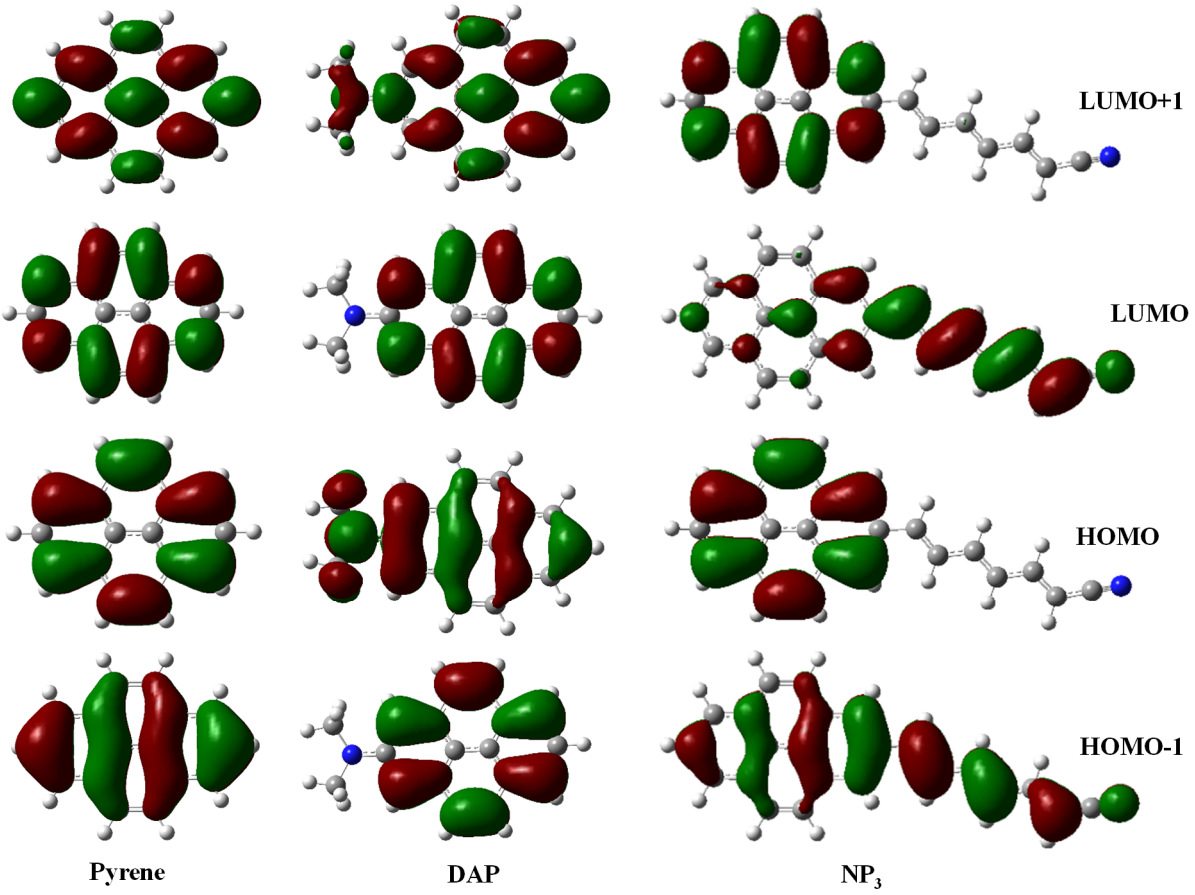


Figure S1. MO diagrams of Pyrene, DAP, and NP_3 molecules in ACN solvent. MO diagrams generated from the optimized geometry using the CAM-B3LYP functional 6-311G++(d,p) basis set considering the CPCM solvation model.