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Computational study on tri-s-triazine-based molecules as ambipolar host materials for phosphorescent blue emitters: effectively geometric and electronic tuning

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Figure SI1 To take insight into this geometric effect, the three conformations of A by fixing the N8-C9-N14-C15 dihedral angles to 30, 60 and 90 degree.

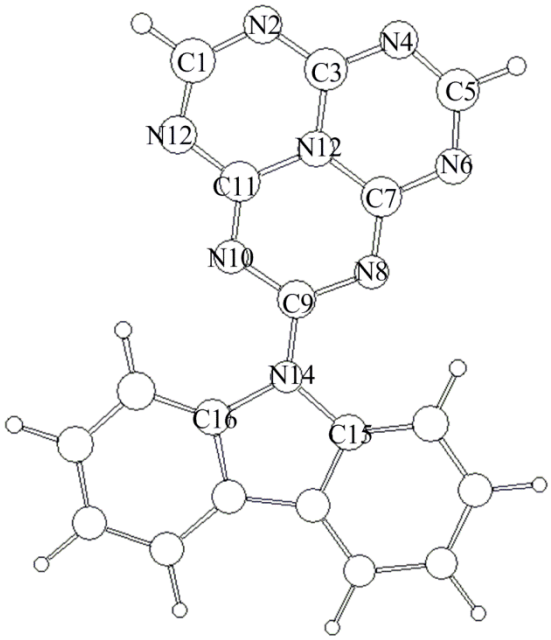

Table SI1 NBO analysis on the ground state and excited state of four conformations of molecule A.

	S0				T1		
Conformation*	Donor NBO	Acceptor NBO	$E^{(2)}$ kcal/mol	Conformation*	Donor NBO	Acceptor NBO	$E^{(2)}$ kcal/mol
plane	LP(1)N14	BD*(2)C9-N10	67.52	plane	LP(1)N14	BD*(2)C9-N10	27.37
30	LP(1)N14	BD*(2)C9-N10	50.96	30	LP(1)N14	BD*(2)C9-N10	--
60	LP(1)N14	BD*(2)C9-N10	6.37	60	LP(1)N14	BD*(2)C9-N10	--
vertical	--	--	--	vertical	--	--	--

*obtained by constraining only the dihedral angle between tri-s-triazine and carbazole planes to 0. 30, 60 and 90 degree.

Table SI2 The E_T values and the energies of HOMO/LUMO and HOMO/LUMO gap for substituted carbazole and tri-s-triazine molecules.

Molecules	E_T	HOMO	LUMO	Eg
Cbz	3.18	-5.44	-0.64	4.80
cbz-F	3.11	-5.55	-1.08	4.47
cbz-CN	3.24	-7.43	-1.71	5.72
cbz-CH_3	3.15	-5.21	-0.60	4.61
cbz-NH_2	2.56	-4.16	-0.32	3.84
tri-s-triazine	2.62	-7.07	-3.16	3.90
tri-s-triazine-NO_2	2.35	-8.17	-4.33	3.84
tri-s-triazine-NH_2	3.05	-6.33	-1.79	4.53
tri-s-triazine-CH_3	2.71	-6.77	-2.76	4.01