Supporting Information

RSC Advances

Theoretical investigation of the anthracene and its derivatives on large energy gap between triplet excited-states

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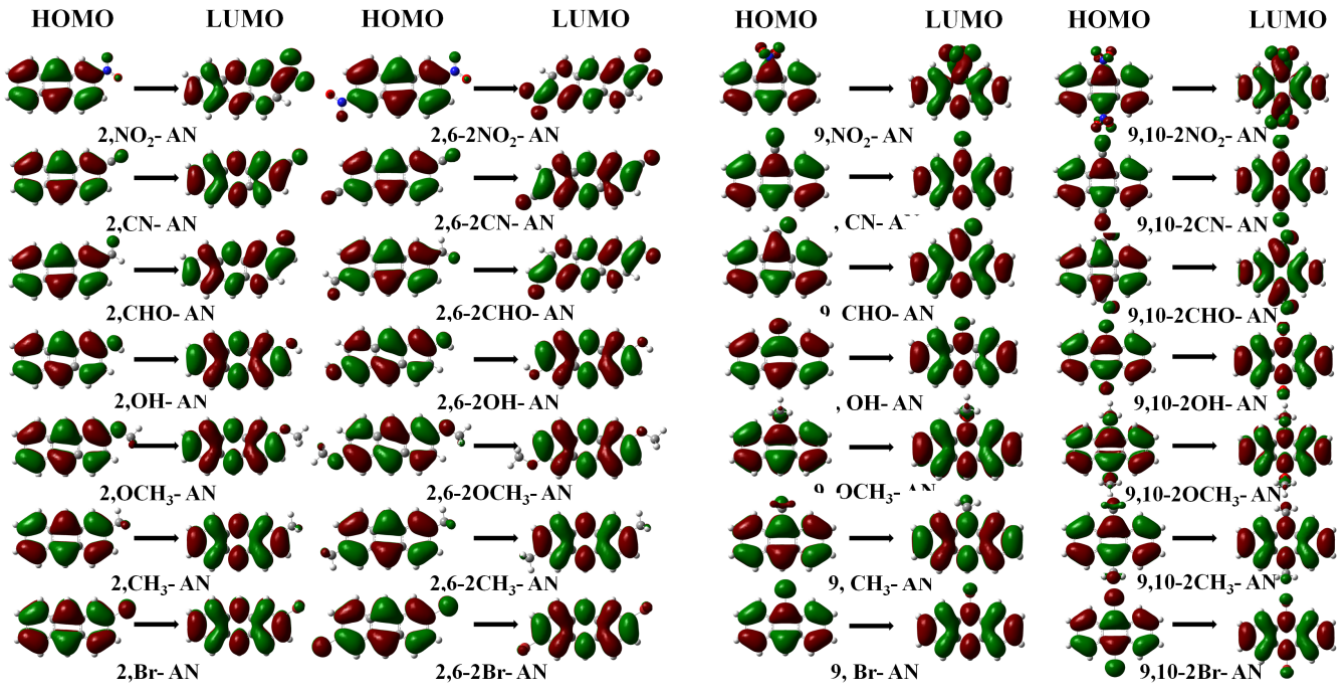
SI-1: The important bond lengths and dihedral angle of anthracene and its derivatives molecules in the ground-state (S_0).

	Distance(Å)		Dihedral angle (°)		Distance(Å)		Dihedral angle (°)
	C1-C2	C9-C12	C1-11-12-10		C1-C2	C9-C12	C1-11-12-10
AN	1.3646	1.4018	180.00	-	1.3646	1.4018	180.00
2,NO_2- AN	1.3692	1.4013	179.99	2,6-2NO_2- AN	1.3685	1.4021	180.00
2,CN-AN	1.3790	1.4012	180.00	2,6-2CN-AN	1.3788	1.4019	179.99
2,CHO- AN	1.3782	1.4025	179.99	2,6-2CHO- AN	1.3782	1.4010	180.00
2,OH- AN	1.3726	1.4021	179.99	2,6-2OH- AN	1.3722	1.4015	179.99
2,OCH_3- AN	1.3763	1.4035	179.97	2,6-2OCH_3- AN	1.3756	1.4020	179.99
2,CH_3-AN	1.3723	1.3999	179.99	2,6-2CH_3-AN	1.3726	1.4017	180.00
2,Br-AN	1.3664	1.4003	179.99	2,6-2Br-AN	1.3666	1.4007	179.99
9,NO_2- AN	1.3675	1.4109	179.20	9,10-2NO_2- AN	1.3675	1.4055	179.97
9,CN-AN	1.3689	1.4169	179.99	9,10-2CN-AN	1.3646	1.4136	179.99
9,CHO- AN	1.3680	1.4298	178.45	9,10-2CHO- AN	1.3690	1.4215	176.72
9,OH- AN	1.3698	1.4109	179.39	9,10-2OH- AN	1.3699	1.4048	178.24
9,OCH_3- AN	1.3694	1.4068	179.85	9,10-2OCH_3- AN	1.3699	1.4060	179.69
9,CH_3-AN	1.3669	1.4052	179.73	9,10-2CH_3-AN	1.3696	1.4031	170.32
9,Br-AN	1.3677	1.4072	179.99	9,10-2Br-AN	1.3678	1.4051	179.99

SI-2: The HOMO and LUMO of anthracene and its derivatives molecules.



SI-3: The energy of HOMO and LUMO of anthracene and its derivatives molecules.

The energy of frontier molecular orbitals (eV)							
	HOMO	LUMO	$\triangle E_{H-L}$		HOMO	LUMO	$\triangle E_{H-L}$
AN	-5.52	-1.97	3.55	-			
2,NO_2- AN	-5.83	-2.61	3.22	2,6-2NO_2- AN	-6.39	-3.27	3.12
2,CN-AN	-5.74	-2.28	3.46	2,6-2CN-AN	-6.22	-2.84	3.38
2,CHO- AN	-5.57	-2.67	2.9	2,6-2CHO- AN	-5.93	-2.74	3.19
2,OH- AN	-5.07	-1.59	3.48	2,6-2OH- AN	-4.89	-1.55	3.34
2,OCH_3- AN	-4.99	-1.57	3.42	2,6-2OCH_3- AN	-4.75	-1.52	3.23
2,CH_3-AN	-5.17	-1.56	3.61	2,6-2CH_3-AN	-5.11	-1.54	3.57
2,Br-AN	-5.45	-1.89	3.56	2,6-2Br-AN	-5.64	-2.12	3.52
9,NO_2- AN	-5.79	-2.48	3.31	9,10-2NO_2- AN	-6.26	-3.07	3.19
9,CN-AN	-5.73	-2.37	3.36	9,10-2CN-AN	-6.23	-2.99	3.24
9,CHO- AN	-5.63	-2.40	3.23	9,10-2CHO- AN	-5.92	-3.05	2.87
9,OH- AN	-4.96	-1.55	3.41	9,10-2OH- AN	-5.08	-1.64	3.44
9,OCH_3- AN	-5.14	-1.63	3.51	9,10-2OCH_3- AN	-5.03	-1.63	3.4
9,CH_3-AN	-5.12	-1.55	3.57	9,10-2CH_3-AN	-5.01	-1.59	3.42
9,Br-AN	-5.39	-1.91	3.48	9,10-2Br-AN	-5.53	-2.16	3.37