

## Effects of Iptycene Scaffolds on the Photoluminescence of *N,N*-Dimethylaminobenzonitrile and Its Analogues

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### Supporting Information (10 pages)

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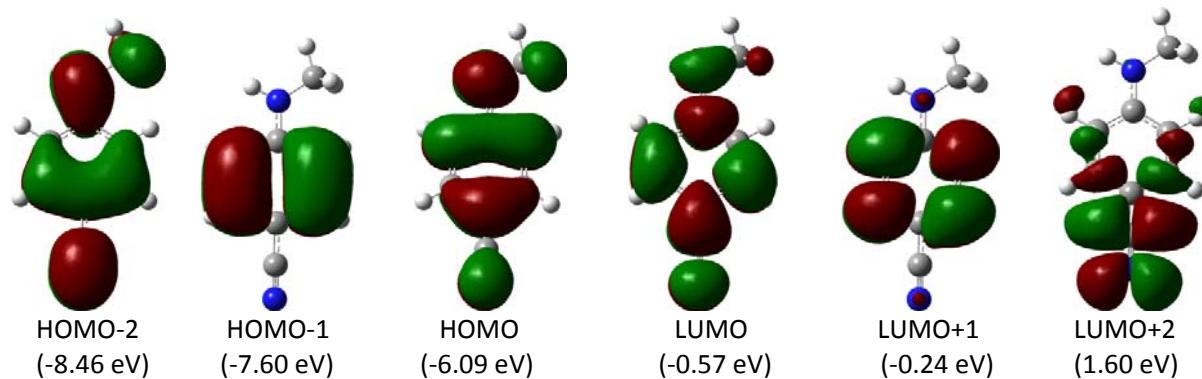
**Table S1.** TDDFT-derived electric transition wavelength ( $\lambda_{\max}$ ) and oscillator strength ( $f$ ) for singlet states  $S_1$  and  $S_2$  of aminobenzonitriles in hexane.

Compd	State	Hexane	
		$\lambda_{\max}$ (nm)	$f$
MABN	$S_1$	268	0.096
	$S_2$	259	0.504
MACT	$S_1$	280	0.011
	$S_2$	268	0.359
MACP	$S_1$	297	0.213
	$S_2$	275	0.082
DMABN	$S_1$	271	0.035
	$S_2$	268	0.616
DMACT	$S_1$	287	0.217
	$S_2$	280	0.084
DMACP	$S_1$	305	0.115
	$S_2$	302	0.197
PABN	$S_1$	299	0.763
	$S_2$	278	0.034
PACT	$S_1$	307	0.627
	$S_2$	290	0.074
PACP	$S_1$	318	0.256
	$S_2$	304	0.147

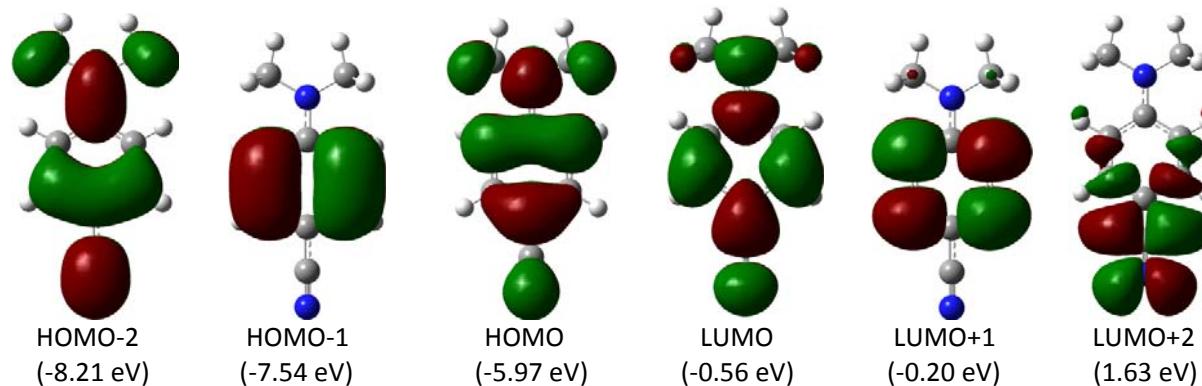
**Table S2.** TDDFT-derived electric transition wavelength ( $\lambda_{\max}$ ) and oscillator strength ( $f$ ) for singlet states  $S_1$  and  $S_2$  of aminobenzonitriles in acetonitrile.

Compd	State	Acetonitrile	
		$\lambda_{\max}$ (nm)	$f$
MABN	$S_1$	269	0.173
	$S_2$	263	0.439
MACT	$S_1$	282	0.011
	$S_2$	272	0.379
MACP	$S_1$	300	0.210
	$S_2$	279	0.111
DMABN	$S_1$	274	0.625
	$S_2$	273	0.031
DMACT	$S_1$	292	0.254
	$S_2$	283	0.043
DMACP	$S_1$	317	0.082
	$S_2$	305	0.208
PABN	$S_1$	303	0.768
	$S_2$	278	0.026
PACT	$S_1$	312	0.620
	$S_2$	292	0.066
PACP	$S_1$	326	0.246
	$S_2$	306	0.137

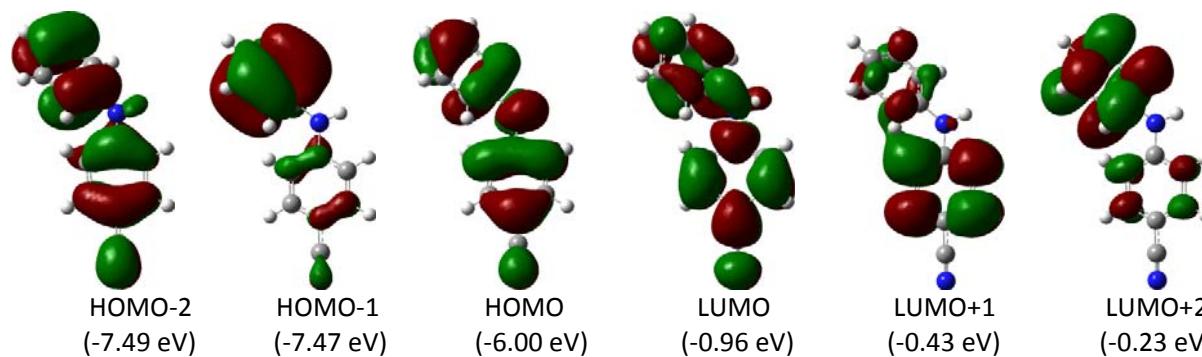
MO diagrams obtained at M06/6-31G\*\* population analysis for M06/6-31G\*\* optimized geometries of **MABN**, **DMABN**, **PABN**, **MACT**, **DMACT**, **PACT**, **MACP**, **DMACP** and **PACP**.



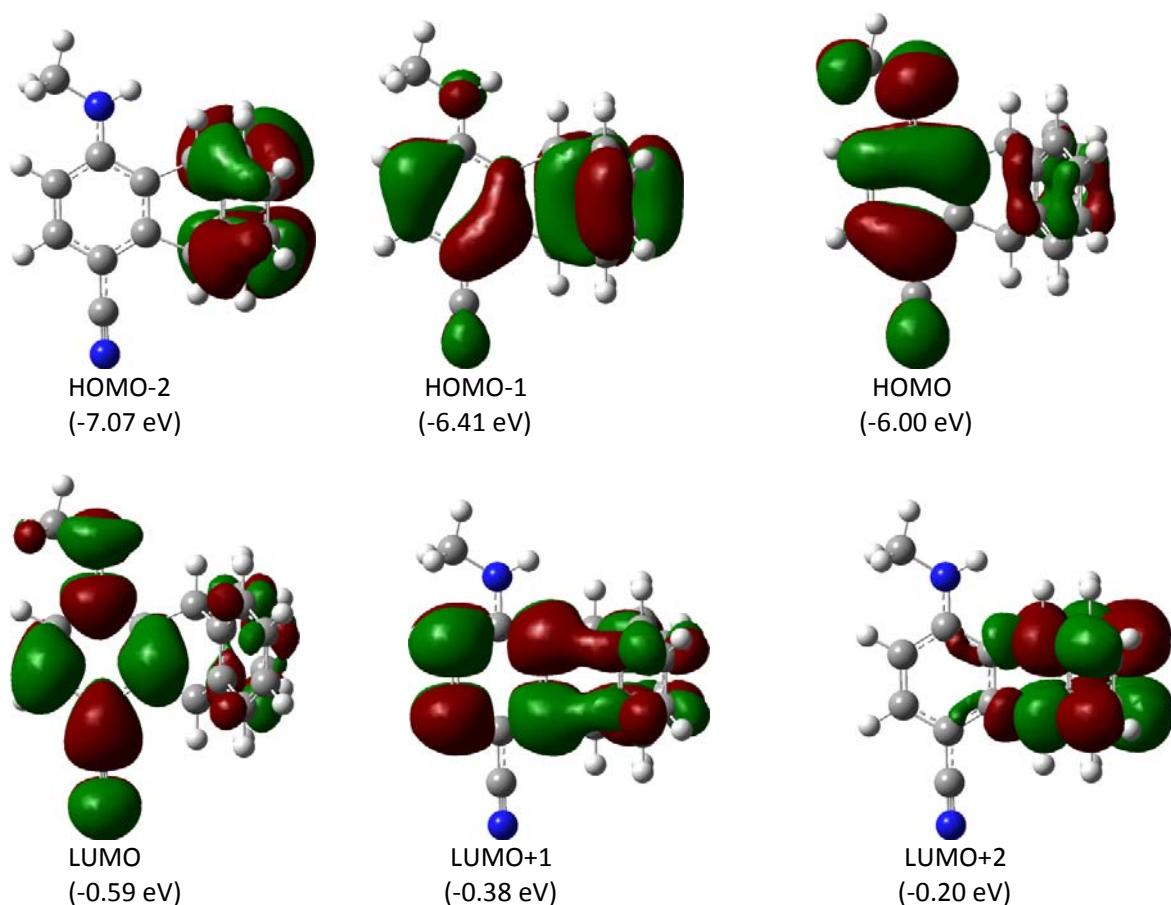
**Figure S1.** MO diagrams of **MABN**



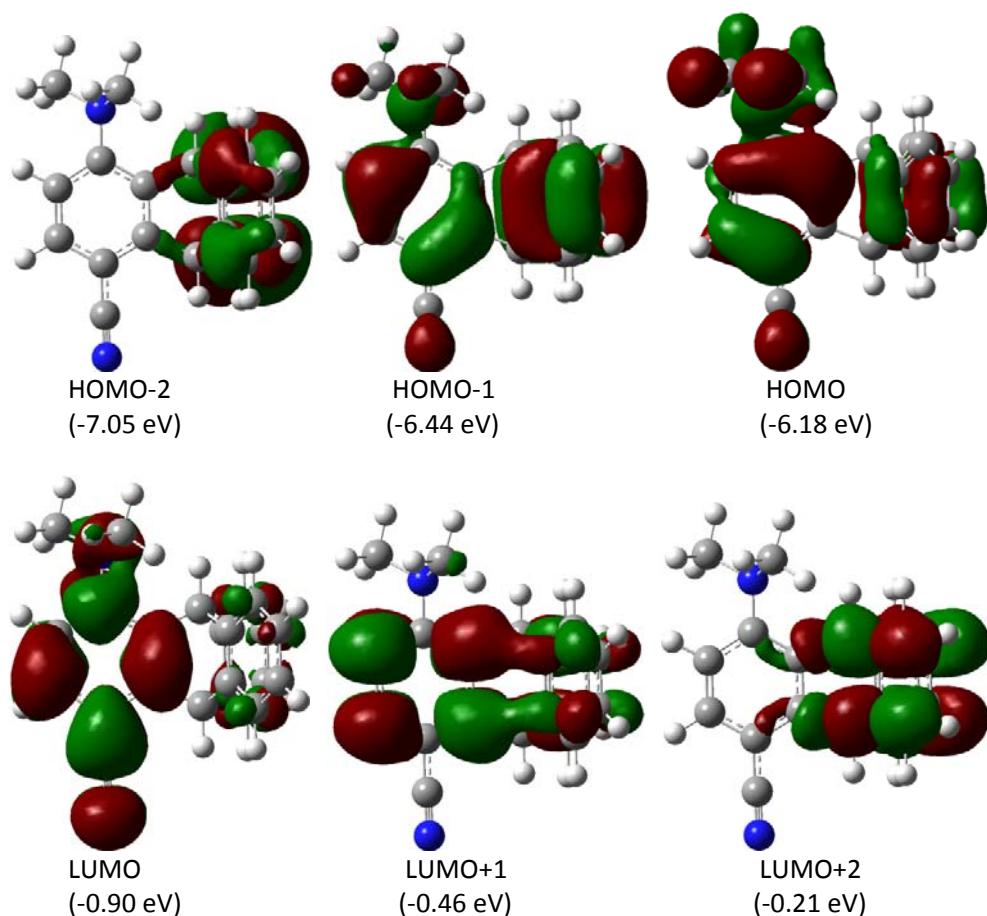
**Figure S2.** MO diagrams of **DMABN**



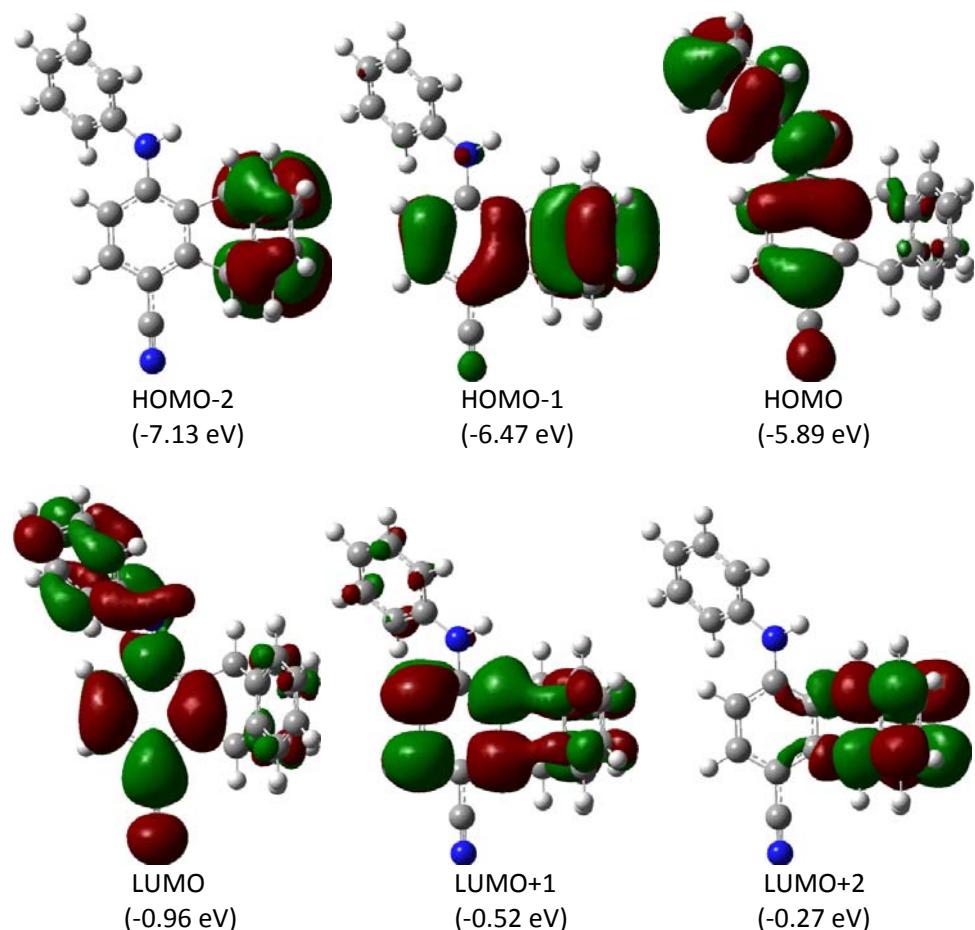
**Figure S3.** MO diagrams of **PABN**



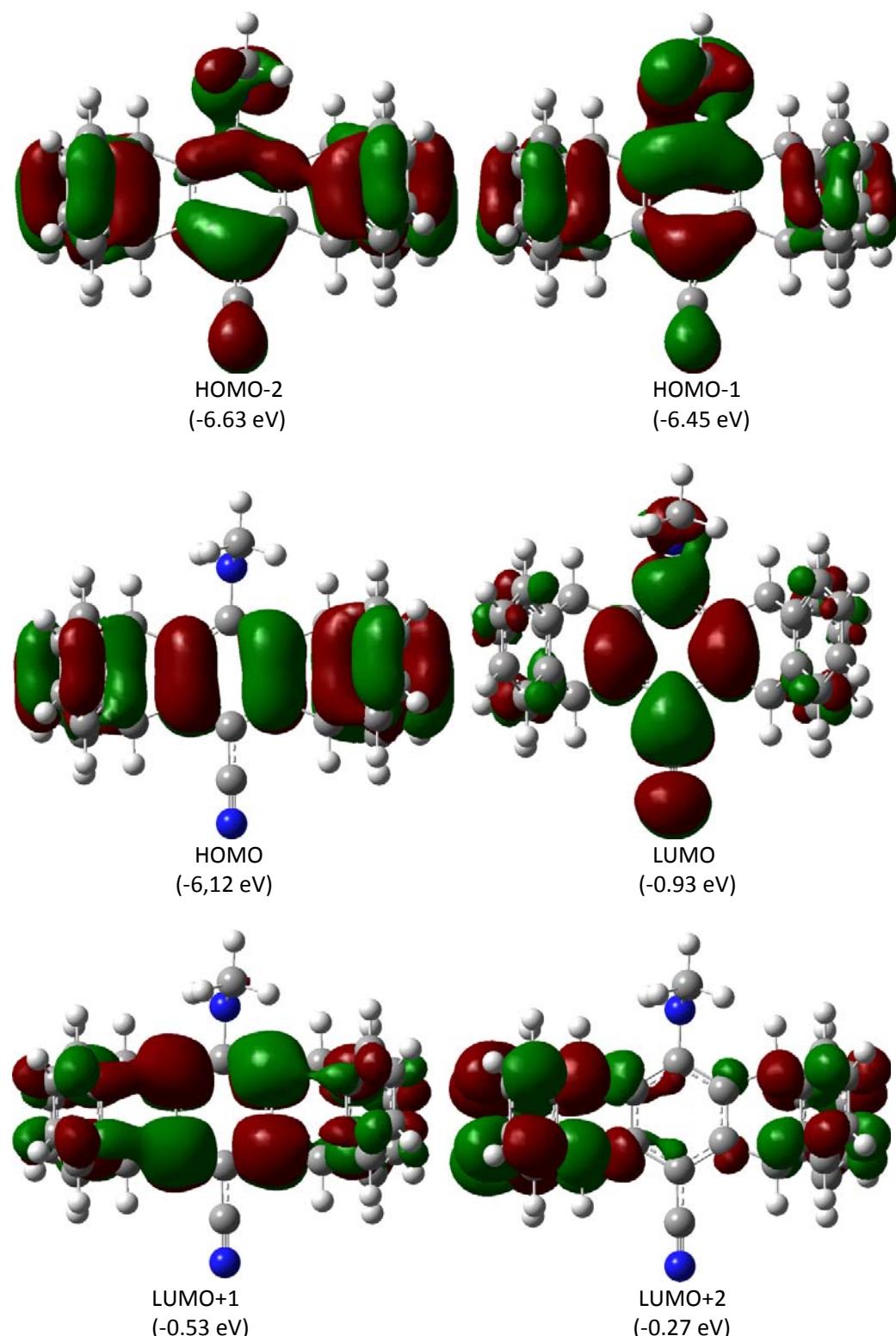
**Figure S4.** MO diagrams of MACT



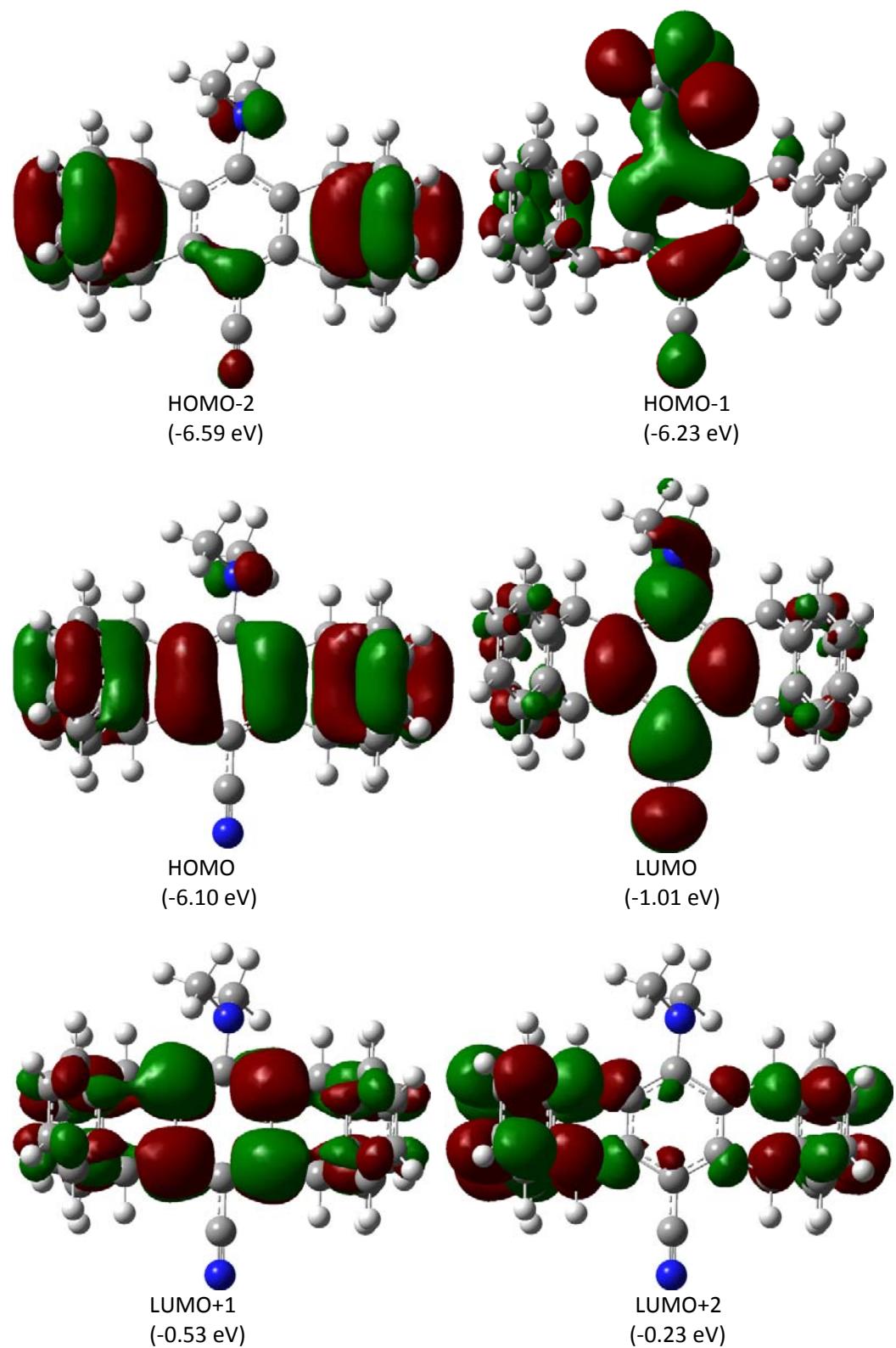
**Figure S5.** MO diagrams of DMACT



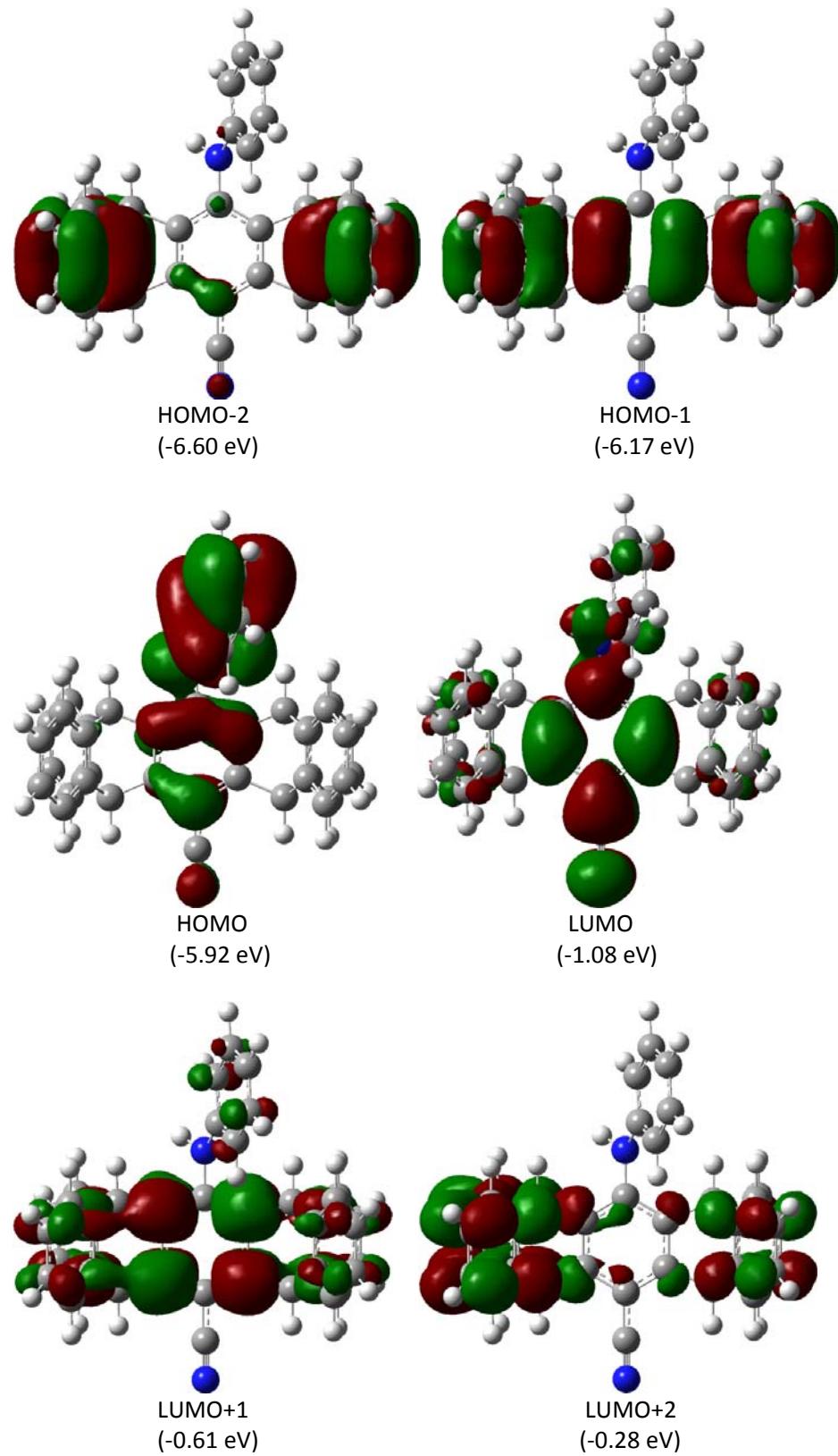
**Figure S6.** MO diagrams of PACT



**Figure S7.** MO diagrams of MACP



**Figure S8.** MO diagrams of DMACP



**Figure S9.** MO diagrams of PACP