Electronic Supplementary Information

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Title: On the formation of sandwich and multidecker complexes via π···π interaction: A DFT study

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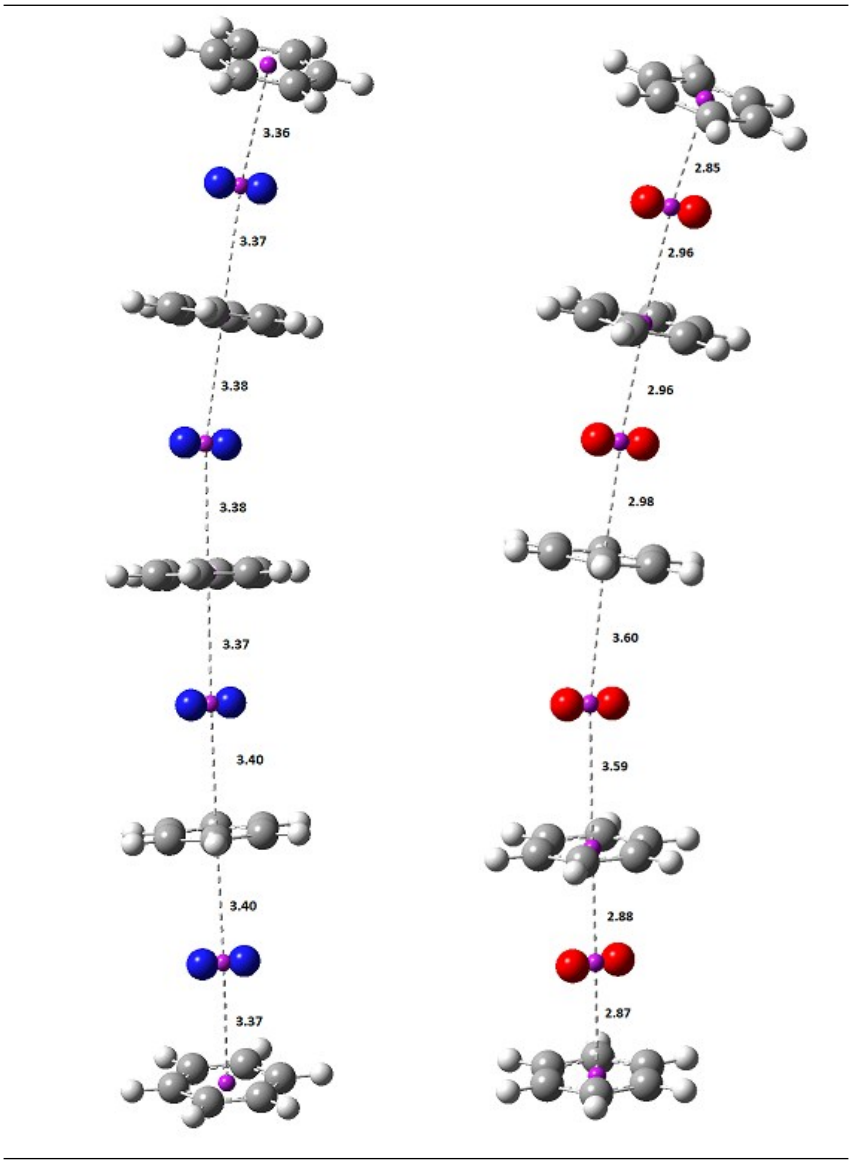

Supplementary Fig. S1: Optimized geometries of (a) 5Ben-4N_2 and (b) 5Ben-4O_2 complexes obtained at ωB97-XD/6-311++G(d,p) level of theory

Supplementary Table S1: λ_{max} (nm), energies (E in eV), oscillators strength (*f*), involved transition and orbital contribution for the complexes obtained at B3LYP/6-31++G(d,p) level of theory

Systems	λ_{max} (nm)	E (eV)	Oscillators strength, *f*	Involved transition	Orbital contribution (%)
Ben	178	6.98	0.61	HOMO−1 → LUMO+1	46.6
				HOMO → LUMO	46.5
Ben-N_2	177	6.99	0.57	HOMO−1 → LUMO+2	46.1
				HOMO → LUMO+3	46.8
	220	5.63	0.05	HOMO → LUMO+1	70.1
Ben-O_2	183	6.77	0.04	HOMO−1 → LUMO+5	69.6
	258	4.80	0.04	HOMO−2 → LUMO	10.9
				HOMO−1 → LUMO+2	69.8
	406	3.05	0.13	HOMO−2 → LUMO	70.3
				HOMO → LUMO+2	10.7
2Ben-N_2	211	5.87	0.11	HOMO → LUMO+2	20.2
				HOMO → LUMO+4	67.2
2Ben-O_2	272	4.56	0.05	HOMO → LUMO+3	20.5
				HOMO → LUMO+4	67.5
	461	2.69	0.25	HOMO−1 → LUMO	70.6
3Ben-2N_2	213	5.81	0.21	HOMO → LUMO+2	52.6
				HOMO → LUMO+4	33.4
3Ben-2O_2	501	2.47	0.47	HOMO−6 → LUMO+1	18.3
				HOMO−3 → LUMO	67.7
4Ben-3N_2	214	5.80	0.18	HOMO−3 → LUMO+3	25.1
				HOMO → LUMO+3	45.7
4Ben-3O_2	523	2.37	0.67	HOMO−8 → LUMO+1	23.4
				HOMO−3 → LUMO	64.8
5Ben-4N_2	216	5.75	0.05	HOMO → LUMO	31.5
				HOMO−1 → LUMO	17.4
5Ben-4O_2	767	1.62	0.001	HOMO−2 → LUMO+1	42.2
				HOMO−2 → LUMO+3	54.0