

Table s1: The selected bond lengths (in Å), bond angles (in degree) and dihedral angles (in degree) of [6,6]PC₇₁BM in gas phase (B3LYP/6-31G(d,p)).

Definition	Value	Definition	Value	Definition	Value
15-71	1.52	14-15-16	103.5	15-5-71-73	-105.1
5-71	1.52	13-14-26	118.4	15-5-71-72	115.5
5-15	1.63	16-15-5	115.4	16-15-5-4	-120.4
71-73	1.52	14-15-5	115.5	73-71-72-74	-179.9
71-72	1.55	15-71-5	64.9	74-80-81-83	-1.6
72-74	1.53	15-71-73	116.0	84-82-81-83	-0.1
81-83	1.21	15-71-72	124.1	80-81-82-84	179.7
81-82	1.35	71-72-74	123.6		
82-84	1.44	82-81-83	123.5		
14-15	1.49	80-81-83	125.7		
15-16	1.49	81-82-84	115.3		

Table s2: the selected bond lengths (in Å), bond angles (in degree) and dihedral angles (in degree) of [5,6]PC₇₁BM in gas phase (B3LYP/6-31G(d,p)).

Definition	Value	Definition	Value	Definition	Value
14-71	1.51	11-12-13	106.1	14-15-71-73	-114.5
15-71	1.51	13-14-26	114.2	14-15-71-72	124.8
14-15	2.13	26-14-15	97.3	26-14-15-5	-119.8
71-73	1.54	13-14-15	108.3	73-71-72-74	178.9
71-72	1.57	14-71-15	89.4	74-80-81-83	3.1
72-74	1.54	14-71-73	112.8	84-82-81-83	0.2
81-83	1.21	14-71-72	120.0	80-81-82-84	-179.6
81-82	1.35	71-72-74	126.2		
82-84	1.44	82-81-83	123.5		
13-14	1.40	80-81-83	125.8		
14-26	1.47	81-82-84	115.3		