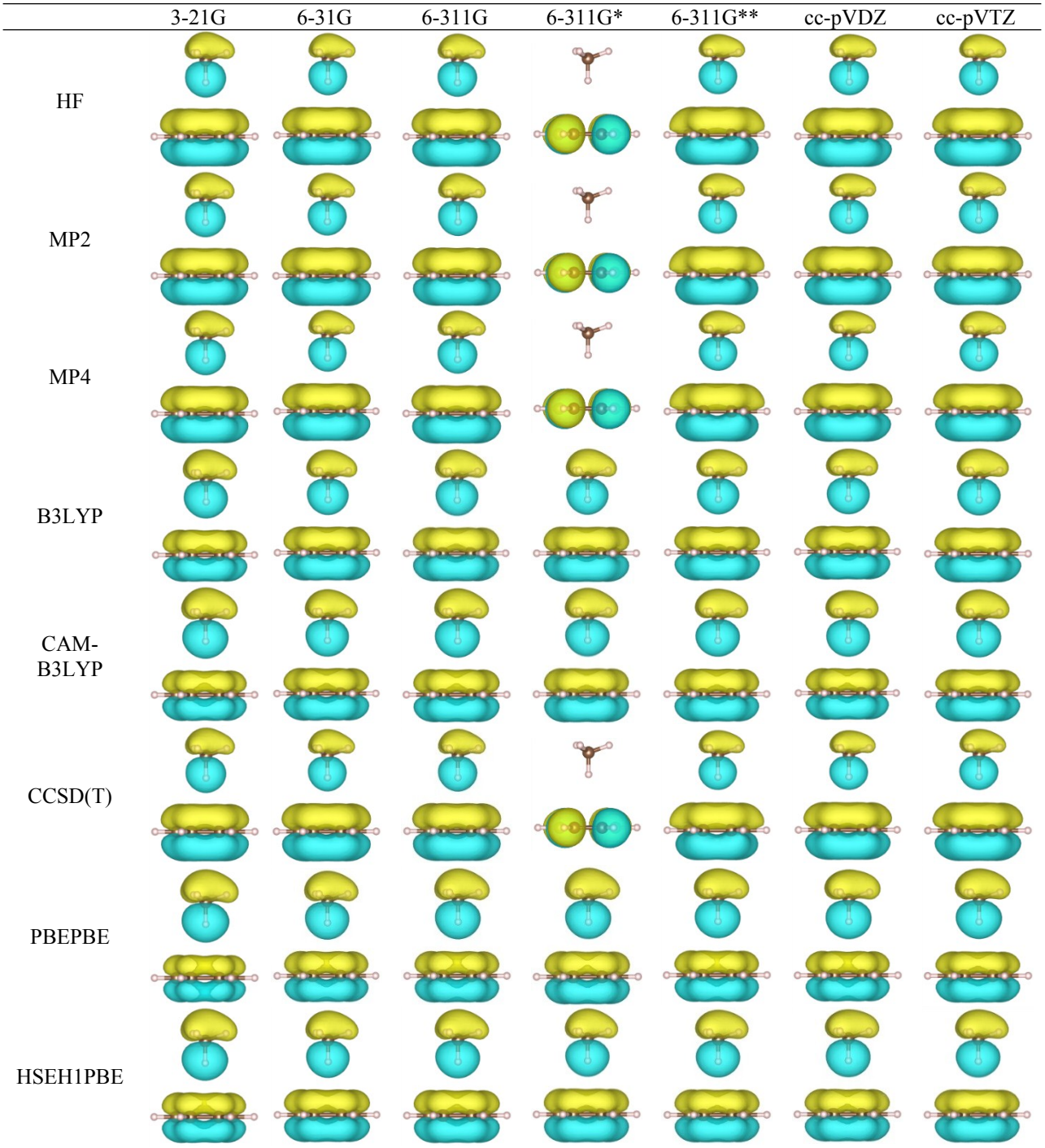
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Supporting Information for the paper entitled “Strong orbital deformation due to CH-π interaction in benzene-methane complex” by Jianfu Li, Rui-Qin Zhang*.



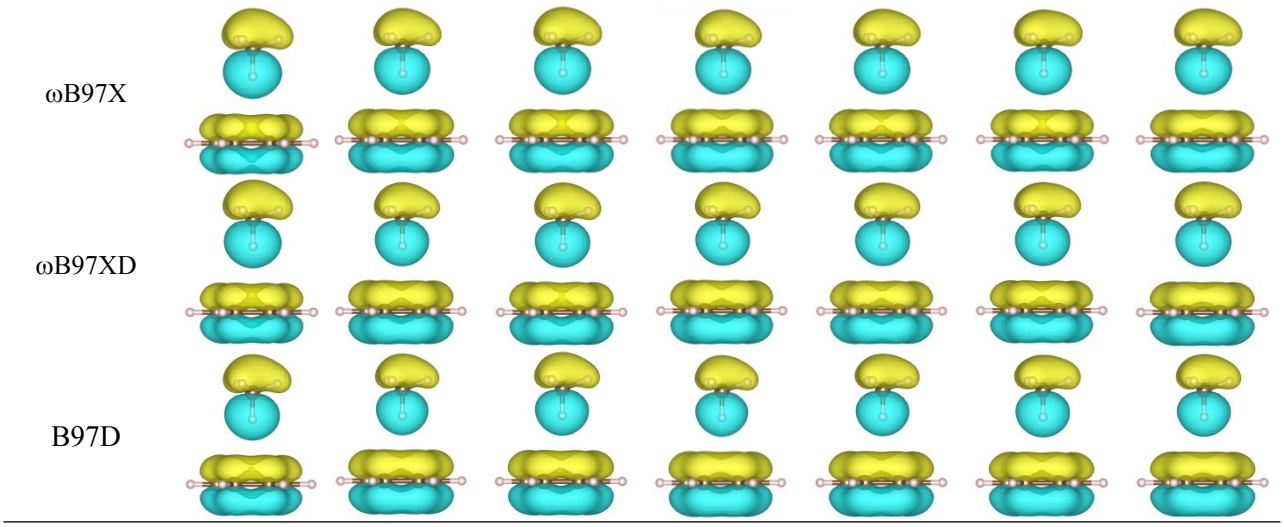


Fig. A1. The HOMO-4 of the benzene-methane complex calculated by using different methods and basis sets. The isosurface value is ±0.03 and the blue and yellow colors denote negative and positive values, respectively.

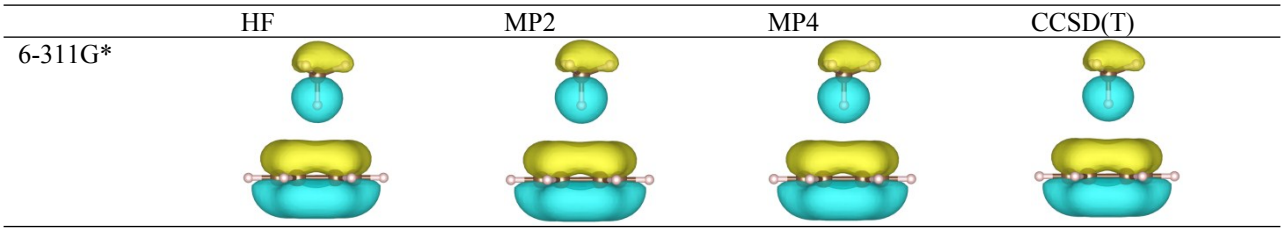


Fig. A2. The HOMO-2 of the benzene-methane complex calculated by using different methods and 6-311G* basis set. The isosurface value is ±0.03 and the blue and yellow colors denote negative and positive values, respectively.

Table A1. The orbital percentage of C_6H_6 for HOMO-4 of the benzene-methane complex calculated using different methods and basis sets. [a] for HOMO-2.

	3-21G	6-31G	6-311G	6-311G*	6-311G**	cc-pVDZ	cc-pVTZ
HF	73	80	78	81[a]	80	80	80
MP2	73	80	78	81[a]	80	80	80
MP4	73	80	78	81[a]	80	80	80
B3LYP	54	67	64	67	65	63	64
CAM-B3LYP	47	59	55	59	57	55	56
CCSD(T)	73	80	78	81[a]	80	80	80
PBEPBE	37	52	49	53	50	47	49
HSEH1PBE	45	60	56	59	57	55	57
ωB97X	40	52	49	52	48	47	49
ωB97XD	43	56	48	56	54	51	53
B97D	53	38	34	37	40	43	41