Supplementary Material for PCCP

Electronic Supplementary information

The Jahn-Teller and pseudo-Jahn-Teller effects in the low-lying electronic states of 1,3,5-trifluorobenzene radical cation

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TABLE I: Normal mode combinations, sizes of the primitive and the single particle basis used in the wave packet propagation within the MCTDH framework in the ($\widetilde{X}$ -$\widetilde{A}$ -$\widetilde{B}$ -$\widetilde{C}$) coupled electronic manifold using the complete vibronic Hamiltonian of Eqs. (2-5e). The CPU time and the required memory of each wave packet calculation are also given.

Normal modes[a]	Primitive basis[b]	SPF basis[c]	CPU time	Required RAM [Mbyte]	Figure
		[$E''_{X,x}$, $E''_{X,y}$, A''_2 $E'_{B,x}$, $E'_{B,y}$, C'_2]			
(ν_2, ν_{11x}, ν_{11y}, ν_{19x}, ν_{19y})	(24, 4, 4, 4, 4)	[8, 8, 8, 8, 8, 4]	$E''_{X,x}$: 24h 33min 37.83s	1094.06	Fig. 6
(ν_{9x}, ν_4, ν_{14y}, ν_{20x}, ν_5)	(18, 5, 5, 4, 4)	[6, 6, 4, 10, 10, 10]	$E''_{X,y}$: 26h 31min 51.55s	1094.06	Fig. 6
(ν_{9y}, ν_{12x}, ν_{14x}, ν_{20y}, ν_{16})	(18, 8, 5, 4, 4)	[6, 6, 4, 8, 8, 4]	A''_2: 16h 43min 59.38s	1094.06	Fig. 6
(ν_{13x}, ν_{12y}, ν_{18x}, ν_3)	(36, 8, 4, 7)	[6, 6, 5, 7, 7, 4]	$E'_{B,x}$: 19h 37min 01.37s	1094.06	Fig. 6
(ν_{13y}, ν_{10x}, ν_{18y}, ν_{10y})	(36, 5, 4, 5)	[7, 7, 4, 6, 6, 5]	$E'_{B,y}$: 22h 09min 42.13s	1094.06	Fig. 6
			C'_2: 22h 08min 00.79s	1094.06	

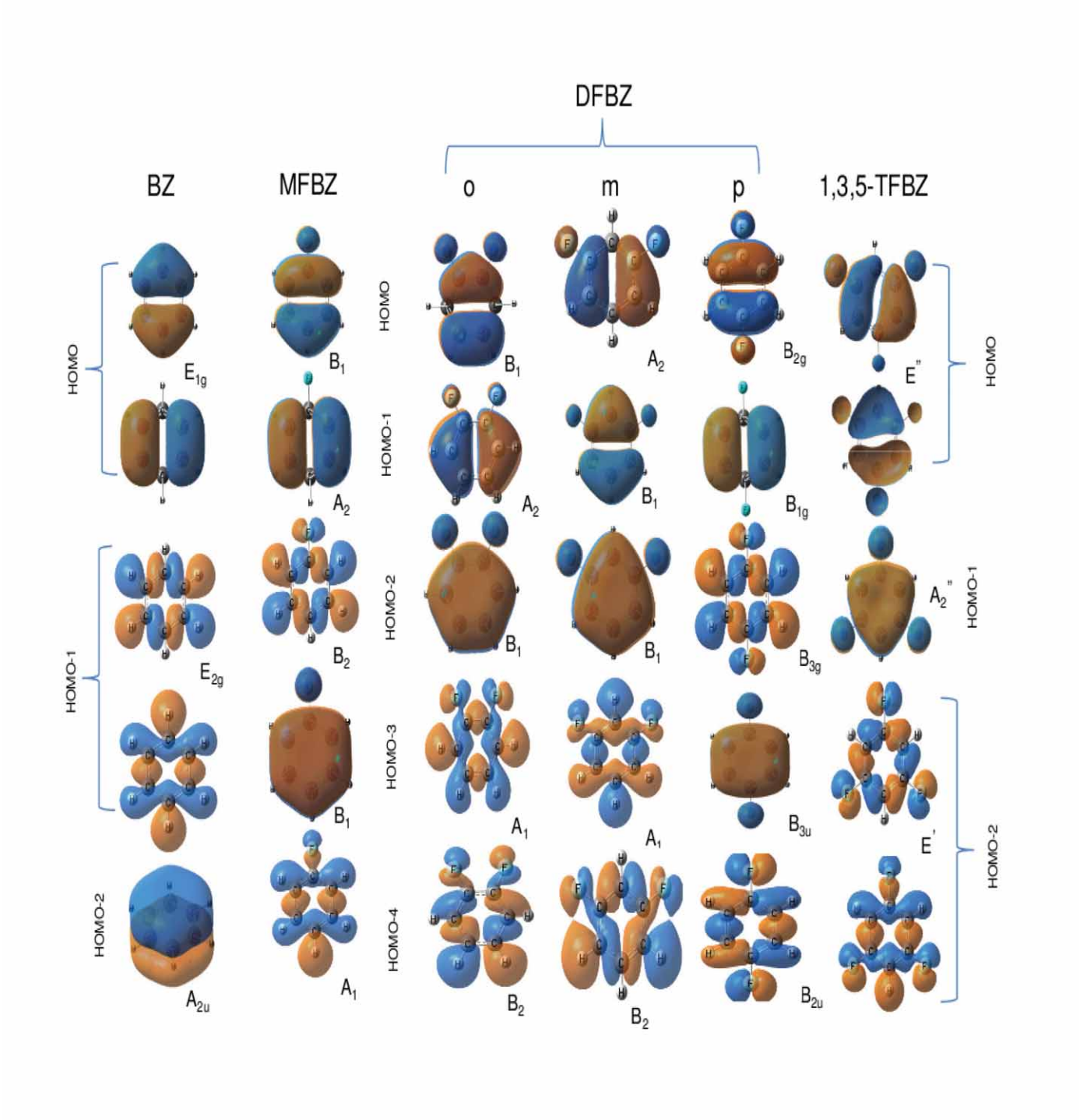

FIG. 1: Schematic plot of the canonical MOs of benzene and its fluoro derivatives. The MOs are calculated at the MP2 level of theory employing cc-pVTZ basis set.