Electronic Supplementary Information

Bonding character, electronic properties, and electronic transitions of perfluorocubane as small electron acceptor

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Table 1. Comparison of the calculated C–C ($R_{C\text{-}C}$, in Å) and C–F ($R_{C\text{-}F}$, in Å) bond lengths, average binding energies (E_b, in eV), and the adiabatic electron affinity (AEA) of the C_8F_8 molecule, obtained by using different functionals and MP2 method.

Methods	Sym.	$R_{C\text{-}C}$	$R_{C\text{-}F}$	E_b	AEA
B3LYP	O_h ($^1A_{1g}$)	1.577	1.338	–4.29	1.78
B3PW91	O_h ($^1A_{1g}$)	1.573	1.334	–4.23	1.71
M062X	O_h ($^1A_{1g}$)	1.569	1.330	–4.30	1.50
TPSSh	O_h ($^1A_{1g}$)	1.577	1.342	–4.21	1.83
MP2	O_h ($^1A_{1g}$)	1.574	1.351	–4.23	1.62
Experiment		1.570	1.341		