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Electron Delocalization and Aromaticity in Low-Lying Excited States of Archetypal Organic Compounds

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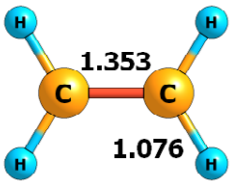
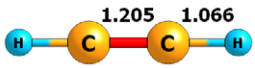
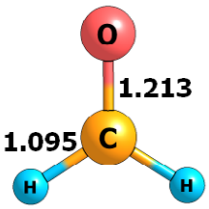
SUPPORTING INFORMATION

Table S1. CASSCF, HF, and B3LYP values of $\delta^{xct}(A,B)$, $\delta^{HF}(A,B)$, and $\delta^{B3LYP}(A,B)$ for the low-lying singlet excited states of C_2H_4, C_2H_2, and CH_2O calculated at the 6-311++g(d,p). All units are in electrons. CASSCF bond distances are given in Å.

Table S2. Values of PDI, FLU, I_{ring}, and MCI for low-lying singlet, triplet, quintet, and septet states of C_6H_6, C_4H_4, and C_8H_8 at the HF/6-311++g(d,p) level of theory. All units are in au.

Table S1. CASSCF, HF, and B3LYP values of $\delta^{xct}(A,B)$, $\delta^{HF}(A,B)$, and $\delta^{B3LYP}(A,B)$ for the low-lying singlet excited states of C_2H_4, C_2H_2, and CH_2O calculated at the 6-311++g(d,p). All units are in electrons. CASSCF bond distances are given in Å.

		$\delta^{xct}(A,B)$	$\delta^{HF}(A,B)$	$\delta^{B3LYP}(A,B)$
C_2H_4 $\delta(C,C)$		1.349	1.885	1.900
C_2H_2 $\delta(C,C)$		1.859	[a]	2.855
CH_2O $\delta(C,O)$		1.243	1.395	1.583

[a] The value of $\delta^{HF}(C,C)$ cannot be calculated due to the presence of non-nuclear attractors.

Table S2. Values of PDI, FLU, I_{ring}, and MCI for low-lying singlet, triplet, quintet, and septet states of C_6H_6, C_4H_4, and C_8H_8 at the HF/6-311++g(d,p) level of theory. All units are in au.

HF	State	PDI	FLU	I_{ring}	MCI
C_6H_6	S_0	0.099	0.000	0.0450	0.0678
D_{6h}	T_1	0.046	0.015	0.0034	-0.002
	Q_1	0.094	0.023	0.0011	0.0423
C_4H_4	S_0		0.098	0.0048	0.0092
D_{2h}	T_1		0.011	0.0349	0.1201
C_8H_8	S_0		0.062	0.0014	0.0008
D_{4h}	T_1		0.004	0.0062	0.0242
	Q_1		0.021	0.0012	0.0075
	$Septet_1$		0.037	0.0000	0.0168