Supporting Information for

How Fluorine Substituents Strengthen Aryl C–H Bonds

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Table S8. Cartesian coordinates (in Å), energies (electronic energy E and enthalpy *H*, in kcal mol^{-1}), number of imaginary frequencies (N_{imag}), and total spin number (*S*) of the equilibrium geometries of all systems studied herein, computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S1. Energy decomposition analysis terms (in kcal mol^{-1}) of the C–H bond for the complete set of substituted benzenes at the equilibrium geometry.[a]

Species	ΔH	$\Delta\Delta H$	$\Delta\Delta H^{b}$	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{disp}	$\Delta E_{spinpol}$
B	–109.3[c]	0.0	0.0	–115.9	1.8	–117.7	–64.9	94.9	–149.5	–0.9	2.7
o	–111.8	–2.5	–2.6	–118.4	1.8	–120.2	–62.0	90.4	–150.5	–0.9	2.8
m	–109.7	–0.4	–0.2	–116.3	1.8	–118.1	–64.1	94.6	–150.4	–0.9	2.7
p	–110.6	–1.3	–1.1	–117.2	1.7	–118.9	–63.5	91.1	–148.2	–1.0	2.7
o-m	–111.8	–2.5	–2.5	–118.3	1.9	–120.2	–61.1	90.3	–151.3	–0.9	2.8
m-p	–110.7	–1.4	–1.1	–117.3	1.8	–119.1	–63.2	91.8	–149.5	–0.9	2.7
2o	–114.8	–5.5	–5.3	–121.1	1.8	–122.9	–58.8	84.3	–150.3	–0.9	2.8
2m	–110.2	–0.9	–0.5	–116.8	1.9	–118.7	–63.0	93.6	–151.0	–1.0	2.7
o-p	–113.0	–3.7	–3.5	–119.5	1.7	–121.2	–60.7	87.0	–149.3	–1.0	2.8
o-m'	–112.2	–2.9	–2.7	–118.7	1.8	–120.5	–61.5	90.7	–151.6	–0.9	2.8
o-m-p	–112.7	–3.4	–3.3	–119.2	1.9	–121.1	–60.2	87.8	–150.5	–1.0	2.8
2m-p	–110.9	–1.6	–1.2	–117.5	1.9	–119.4	–62.4	91.7	–150.5	–0.9	2.7
2o-m	–114.7	–5.4	–5.3	–121.1	1.8	–122.9	–58.4	85.0	–151.5	–0.9	2.9
o-2m	–112.4	–3.1	–2.8	–118.9	1.9	–120.8	–60.2	89.4	–151.8	–1.0	2.8
o-m-p'	–113.1	–3.8	–3.6	–119.6	1.8	–121.4	–60.5	88.0	–150.7	–1.0	2.8
2o-p	–115.7	–6.4	–6.1	–122.1	1.7	–123.8	–57.6	81.3	–149.2	–1.0	2.7
o-2m-p	–113.0[c]	–3.7	–3.5	–119.5	1.9	–121.4	–59.5	87.8	–151.6	–1.0	2.9
2o-2m	–115.0	–5.7	–5.4	–121.3	1.9	–123.2	–57.2	83.7	–151.6	–1.0	2.9
2o-m-p	–115.5	–6.2	–6.0	–121.8	1.8	–123.6	–57.4	82.7	–150.8	–1.0	2.9
2o-2m-p	–115.5[c]	–6.2	–6.0	–121.8	1.9	–123.7	–56.4	82.4	–151.6	–1.0	2.9

[a] Computed at ZORA-BLYP-D3(BJ)/TZ2P level of theory. [b] Relative C–H bond enthalpies reported in reference 4a and computed at B3PW91/6-31G(d,p) level of theory. [c] Experimental values for **B**, **o-2m-p**, and **2o-2m-p** are –113.2, –115.0, and –116.5 kcal mol^{-1}, respectively.[27]

Table S2. Energy decomposition analysis terms (in kcal mol^{-1}) of the C–H bond for substituted benzenes at a consistent geometry[a] with a C–H distance of 1.088 Å.[b] Energies relative to benzene (**B**) for polyfluorinated benzenes are shown in Figure S2.

Species	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	$\Delta E_{oi,\sigma}$	$\Delta E_{oi,\pi}$	ΔE_{disp}	$\Delta E_{spinpol}$
B	–117.7	–64.9	94.9	–149.5	–148.0	–1.6	–0.9	2.7
o	–120.2	–61.9	90.1	–150.2	–148.8	–1.4	–1.0	2.8
m	–118.1	–64.1	94.5	–150.3	–148.9	–1.5	–0.9	2.7
p	–118.9	–63.5	90.8	–148.0	–146.6	–1.4	–0.9	2.7
2o	–122.9	–58.7	83.6	–149.7	–148.6	–1.1	–0.9	2.8
2m	–118.7	–63.0	93.3	–150.8	–149.4	–1.4	–0.9	2.7
2o-p	–123.8	–57.5	80.5	–148.5	–147.5	–1.0	–1.0	2.7
2m-p	–119.4	–62.3	91.2	–150.1	–148.8	–1.3	–0.9	2.7
2o-2m	–123.2	–57.1	83.1	–151.1	–150.2	–1.0	–1.0	2.9
2o-2m-p	–123.7	–56.3	81.8	–151.0	–150.1	–0.9	–1.0	2.8

[a] The C–H equilibrium distance for benzene. [b] Computed at ZORA-BLYP-D3(BJ)/TZ2P level of theory.

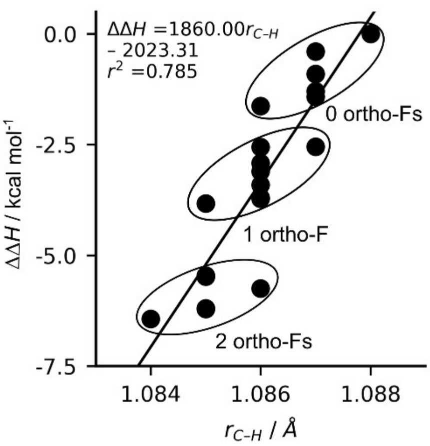


Figure S1. Linear correlation between $\Delta\Delta H$ and the C–H bond lengths. Computed at ZORA-BLYP-D3(BJ)/TZ2P.

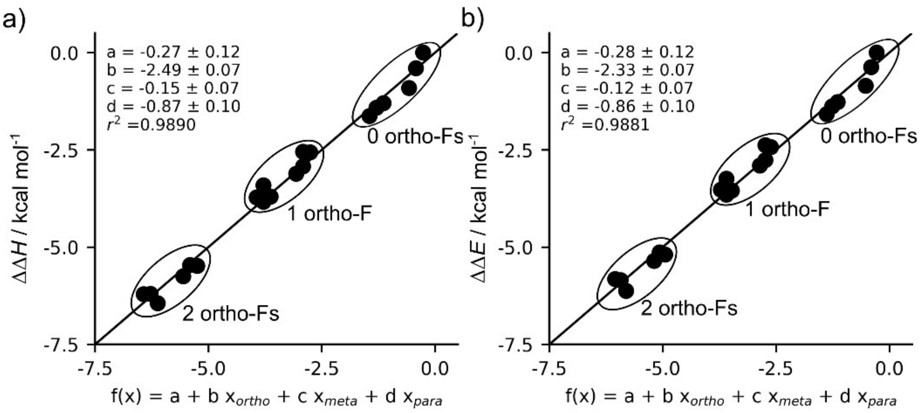


Figure S2. Multiple linear regression relating the number of fluorine substituents at the *ortho*, *meta*, and *para* positions to relative a) C–H bond enthalpies $\Delta\Delta H$ and b) C–H bond energies $\Delta\Delta E$.

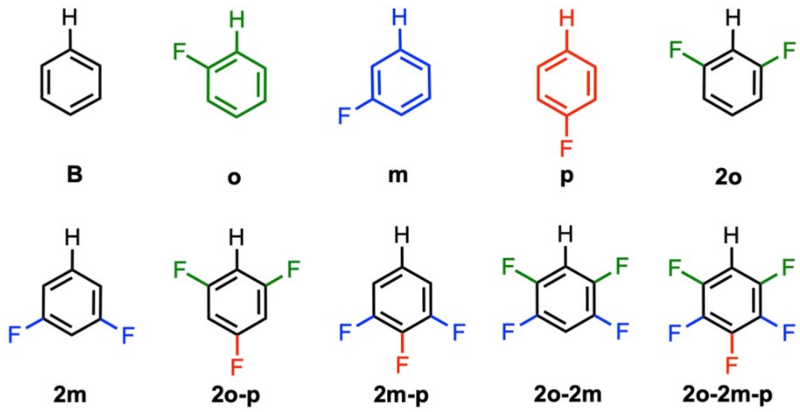
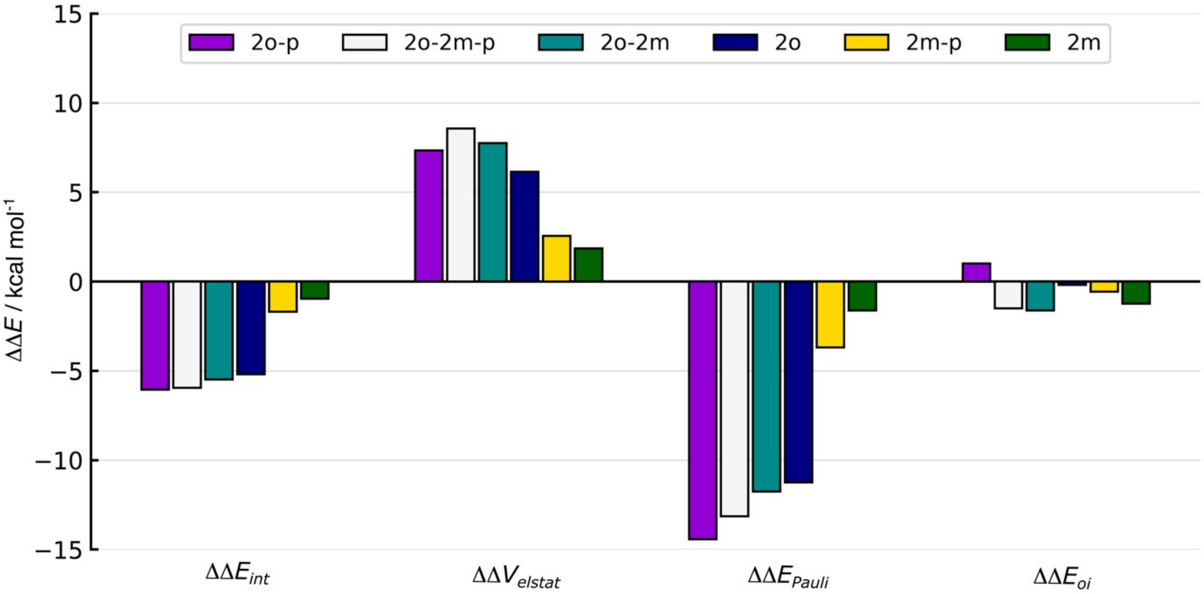


Figure S3. Subset of fluorinated benzenes C_6R_5H (R = H, F) used in both analyses at the consistent-geometry (Table S2) and as a function of the C–H bond distance (Figure S5 and S6).



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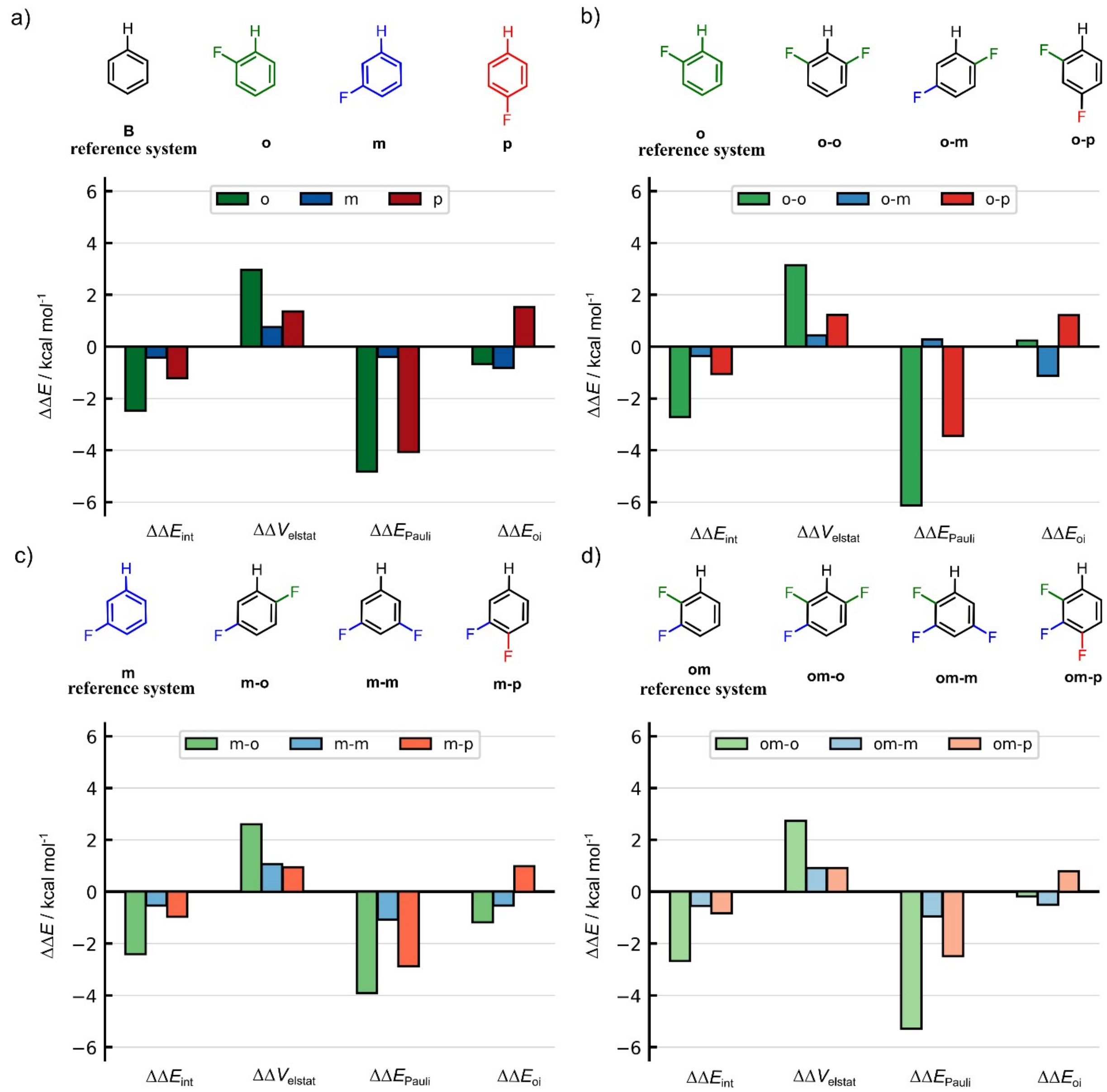

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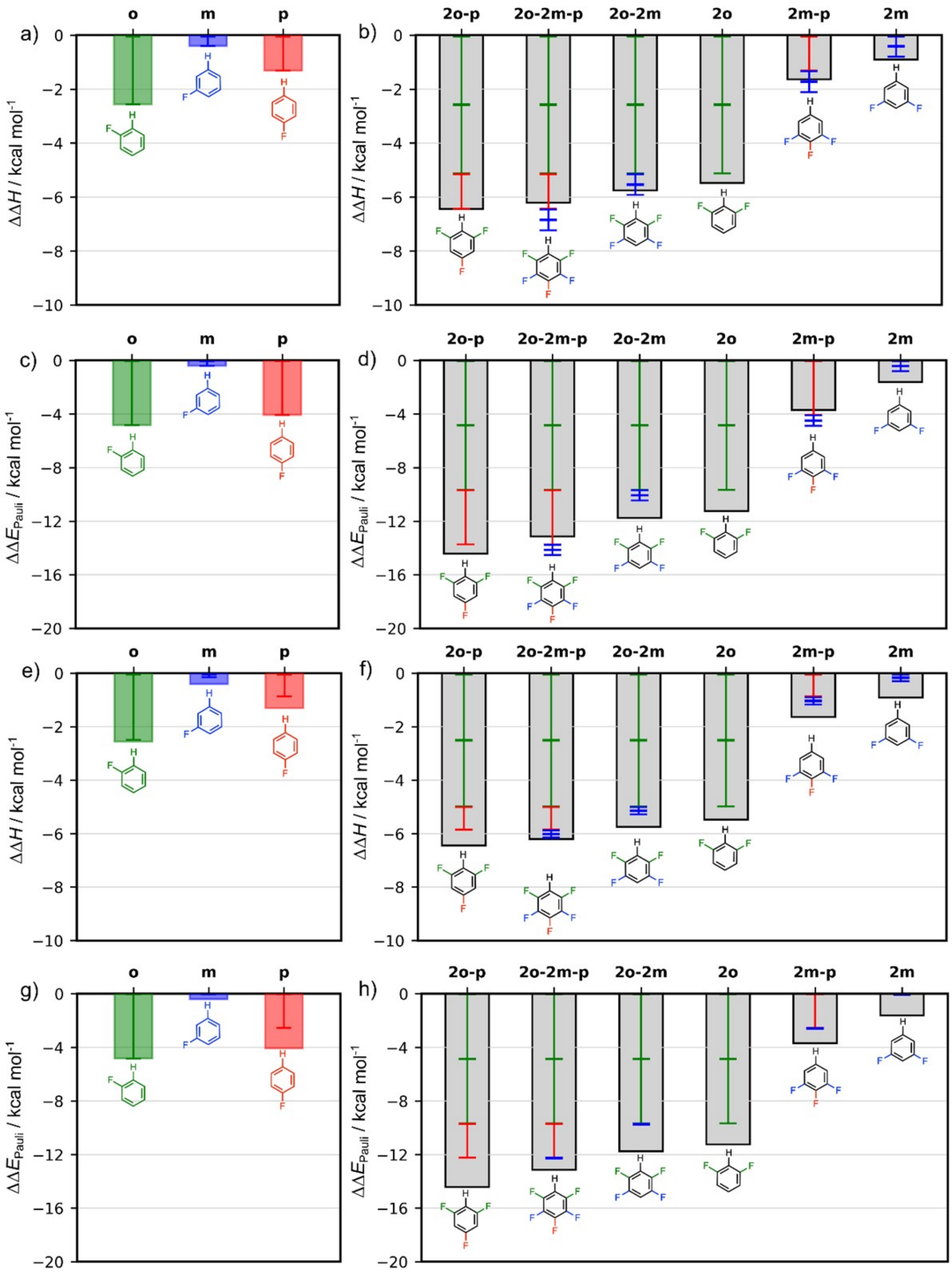


Figure S6. C–H bond enthalpies (colored and gray bars), referenced to the corresponding monosubstituted values (indicated by the vertical lines within the bars), for (a) fluorobenzene and (b) polyfluorinated benzenes. Pauli repulsion terms (colored and gray bars), referenced to the corresponding monosubstituted values, for (c) fluorobenzene and (d) polyfluorinated benzenes. C–H bond enthalpies (colored and gray bars), referenced to the regression coefficients, for (e) fluorobenzene and (f) polyfluorinated benzenes. Pauli repulsion terms (colored and gray bars), referenced to the regression coefficients, for (g) fluorobenzene and (h) polyfluorinated benzenes. Computed at ZORA-BLYP-D3(BJ)/TZ2P. All values relative to those in benzene.

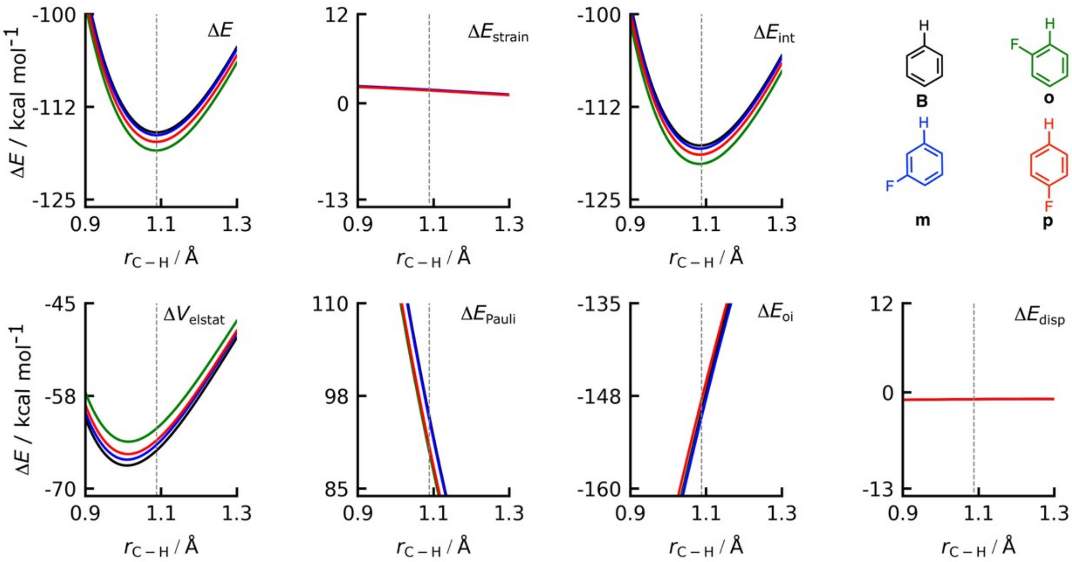
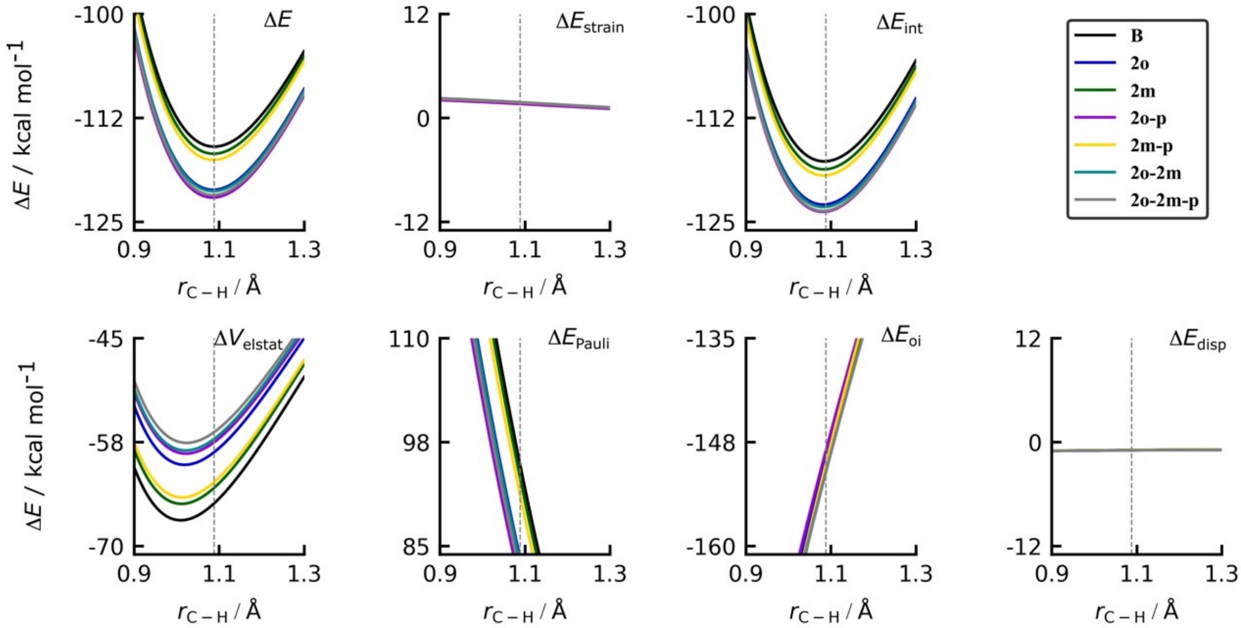


Figure S7. Energy decomposition analysis terms as a function of the C–H bond distance in benzene and fluorobenzene. The dashed vertical line indicates the consistent geometry with a C–H bond distance of 1.088 Å. Computed at ZORA-BLYP-D3(BJ)/TZ2P.



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Orbital	System	*S*	Δ*S*	Orbital	System	*S*	Δ*S*
σ_{SOMO}	**B**	0.61	0.00	$\sigma_{HOMO\text{-}7}$	**B**	0.18	0.00
	o	0.61	0.00		**o**	0.16	−0.02
	m	0.60	−0.01		**m**	0.16	−0.02
	p	0.61	0.00		**p**	0.17	−0.01
$\sigma_{HOMO\text{-}2}$	**B**	0.21	0.00	$\sigma_{HOMO\text{-}9}$	**B**	0.28	0.00
	o	0.16	−0.05		**o**	0.23	−0.05
	m	0.17	−0.04		**m**	0.25	−0.03
	p	0.20	−0.01		**p**	0.27	−0.01
$\sigma_{HOMO\text{-}5}$	**B**	0.07	0.00	$\sigma_{HOMO\text{-}11}$	**B**	0.21	0.00
	o	0.09	0.02		**o**	0.20	−0.01
	m	0.05	−0.02		**m**	0.21	0.00
	p	0.16	0.09		**p**	0.21	0.00
$\sigma_{HOMO\text{-}6}$	**B**	0.18	0.00	$\sigma_{HOMO\text{-}17}$	**B**	0.08	0.00
	o	0.12	−0.06		**o**	0.08	0.00
	m	0.19	0.01		**m**	0.08	0.00
	p	0.09	−0.09		**p**	0.08	0.00

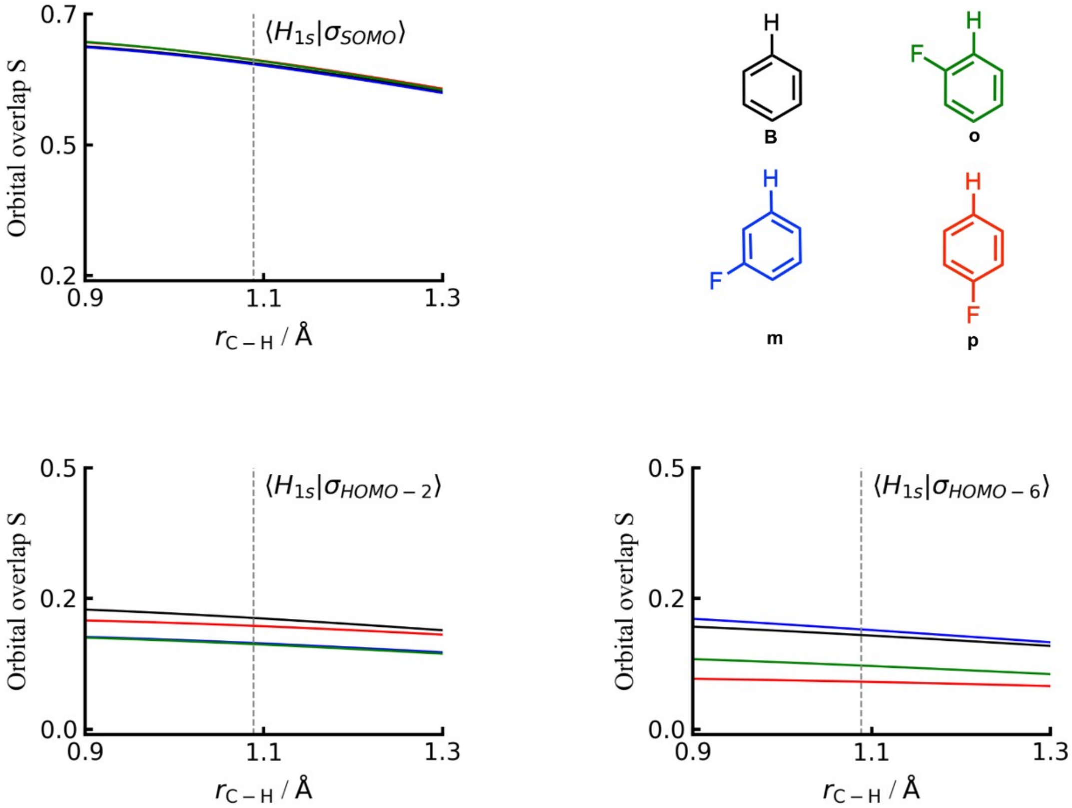


Figure S9. Orbital overlaps as a function of the C–H bond distance in benzene and fluorobenzene computed at ZORA-BLYP-D3(BJ)/TZ2P.

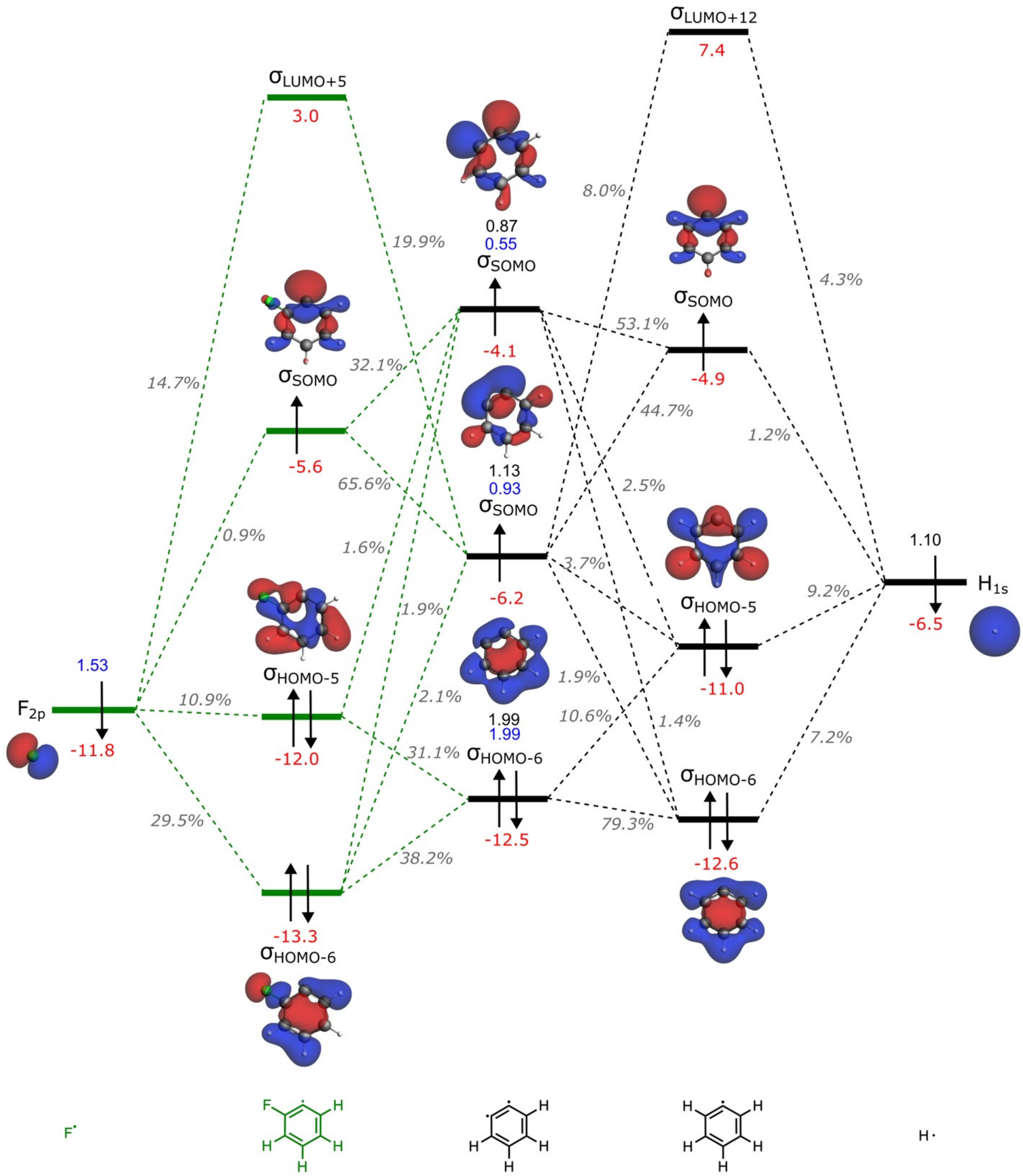
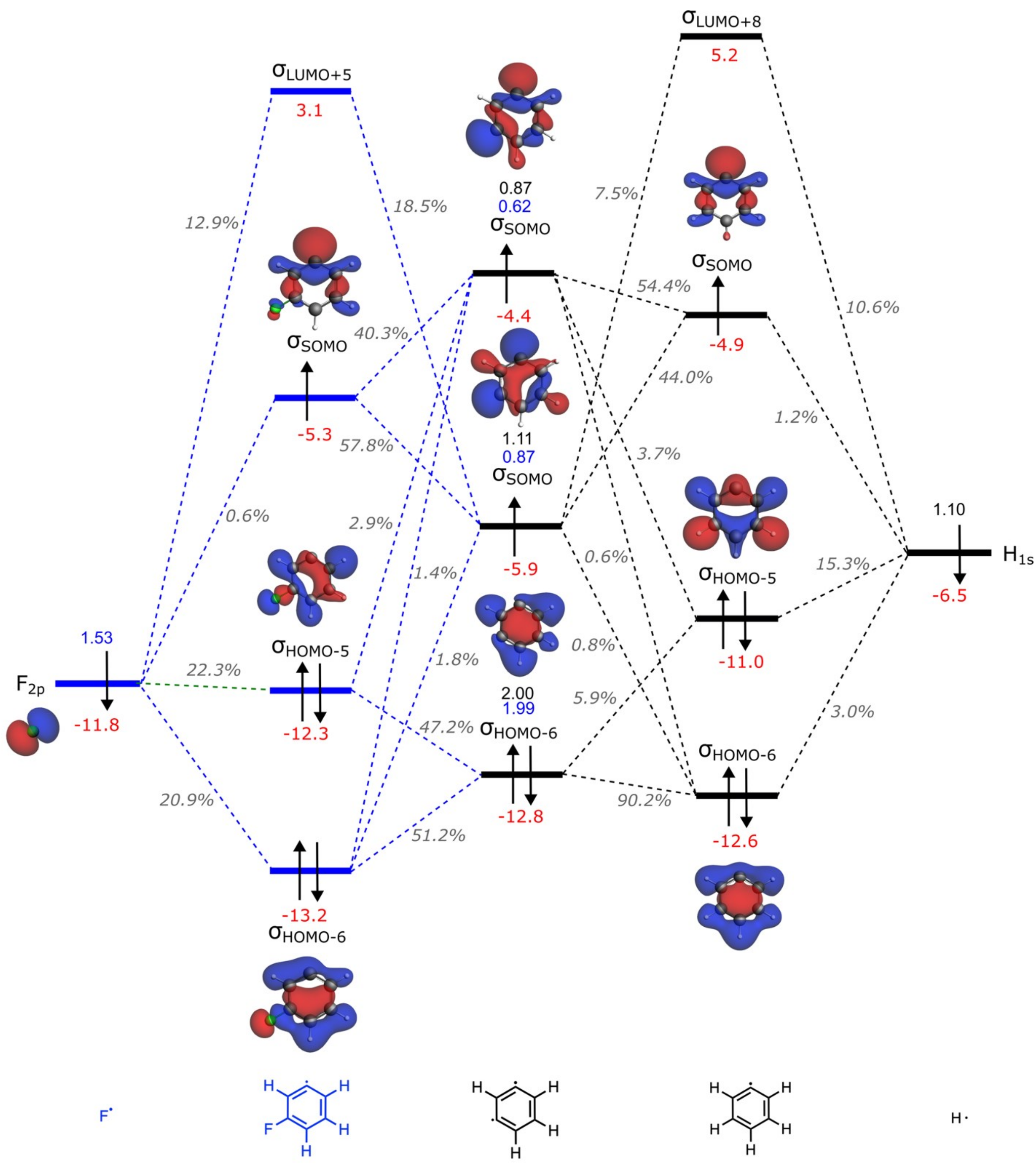


Figure S10. Qualitative MO diagram showing the formation of the σ_{SOMO} and $\sigma_{HOMO\text{-}6}$ of the *ortho*-aryl radical ($C_6H_4R^{\bullet}$) from the interaction of $C_6H_4^{\bullet\bullet}$ + $R^{\bullet}$ (R = F *versus* H). The orbital energies (in eV) are given in red, gross population (in electrons) in blue (R = F) and black (R = H), and SFO Gross Mulliken contributions in gray. Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S4. SFO Gross Mulliken contributions (%)[a] to the MOs of the *ortho*-aryl radical ($C_6H_4R^•$) formed from the interaction of $C_6H_4^{••}$ + $R^•$ (R = F or H). Computed at ZORA-BLYP-D3(BJ)/TZ2P.

MO	SFO Gross Mulliken contributions (%)	
	R = F	R = H
σ_{SOMO}	65.6% σ_{HOMO-1} 32.1% σ_{HOMO}	53.1% σ_{HOMO} 44.7% σ_{HOMO-1} 1.2% H_{1s}
σ_{HOMO-1}	39.0% σ_{HOMO-3} 25.8% σ_{HOMO-2} 17.0% F_{2px}[b] 5.7% σ_{HOMO-5} 4.3% σ_{HOMO-1} 2.8% F_{2pz}[c] 2.3% σ_{HOMO}	48.6% σ_{HOMO-2} 19.0% σ_{HOMO-1} 10.8% σ_{HOMO-3} 10.0% H_{1s} 7.5% σ_{HOMO} 1.9% σ_{HOMO-6} 1.0% σ_{HOMO-4}
σ_{HOMO-2}	49.9% σ_{HOMO-3} 22.6% σ_{HOMO-2} 14.5% F_{2px}[b] 10.0% σ_{HOMO-5}	51.5% σ_{HOMO-3} 38.6% σ_{HOMO-2} 3.2% σ_{HOMO-1} 3.2% H_{1s} 1.5% σ_{HOMO}
σ_{HOMO-3}	89.3% σ_{HOMO-4} 2.8% F_{2pz}[c] 2.3% σ_{HOMO-3} 1.8% σ_{HOMO-6} 1.1% σ_{HOMO-2}	37.9% σ_{HOMO-4} 27.1% σ_{HOMO-3} 10.3% H_{1s} 7.8% σ_{HOMO-2} 5.5% σ_{HOMO-6} 5.4% σ_{HOMO-1} 3.3% σ_{HOMO} 1.5% σ_{HOMO-7}
σ_{HOMO-4}	47.2% σ_{HOMO-5} 26.0% σ_{HOMO-6} 8.9% F_{2px}[b] 5.8% F_{2pz}[c] 3.0% σ_{HOMO-4} 2.9% σ_{HOMO-2} 2.2% σ_{HOMO} 1.0% σ_{HOMO-8}	99.5% σ_{HOMO-5}
σ_{HOMO-5}	31.1% σ_{HOMO-6} 30.4% σ_{HOMO-5} 10.9% F_{2pz}[c] 7.1% F_{2px}[b] 5.1% σ_{HOMO-7} 5.0% σ_{HOMO-4} 4.1% σ_{HOMO-3} 2.2% σ_{HOMO-1} 1.7% σ_{HOMO}	59.4% σ_{HOMO-4} 10.6% σ_{HOMO-6} 9.2% H_{1s} 8.2% σ_{HOMO-3} 3.7% σ_{HOMO-1} 3.0% σ_{HOMO-2} 2.5% σ_{HOMO} 1.8% σ_{HOMO-7}
σ_{HOMO-6}	38.2% σ_{HOMO-6} 29.5% F_{2pz}[c] 13.8% σ_{HOMO-7} 3.5% σ_{HOMO-8} 2.5% F_{2s} 2.1% σ_{HOMO-1} 1.9% σ_{HOMO} 1.6% σ_{HOMO-9} 1.5% σ_{HOMO-3} 1.1% σ_{HOMO-4}	79.3% σ_{HOMO-6} 7.2% H_{1s} 5.0% σ_{HOMO-7} 2.0% σ_{HOMO-1} 1.4% σ_{HOMO} 1.4% σ_{HOMO-8} 1.0% σ_{HOMO-3}

[a] Only contributions greater than 1% are listed. [b] doubly occupied orbital. [c] F_{2pz} corresponds to the SOMO of the fluorine.



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MO	SFO Gross Mulliken contributions (%)	
	R = F	R = H
σ_{SOMO}	57.8% σ_{HOMO-1} 40.3% σ_{HOMO}	54.4% σ_{HOMO} 44.0% σ_{HOMO-1} 1.2% H_{1s}
σ_{HOMO-1}	56.3% σ_{HOMO-2} 30.4% F_{2px}[b] 3.8% σ_{HOMO-3} 2.4% σ_{HOMO} 1.7% σ_{HOMO-1} 1.7% F_{2pz}[c] 1.3% σ_{HOMO-4} 1.0% σ_{HOMO-3}	49.8% σ_{HOMO-2} 18.3% σ_{HOMO-1} 10.8% σ_{HOMO-3} 9.9% H_{1s} 7.8% σ_{HOMO} 1.4% σ_{HOMO-7}
σ_{HOMO-2}	67.8% σ_{HOMO-3} 16.4% σ_{HOMO-2} 7.8% σ_{HOMO-5} 7.0% F_{2px}[b]	67.8% σ_{HOMO-3} 28.9% σ_{HOMO-2} 1.0% σ_{HOMO-1}
σ_{HOMO-3}	92.9% σ_{HOMO-4} 1.6% F_{2pz}[c] 1.4% σ_{HOMO-2} 1.0% σ_{HOMO-5}	50.3% σ_{HOMO-4} 13.9% σ_{HOMO-3} 11.3% σ_{HOMO-2} 10.2% H_{1s} 5.7% σ_{HOMO-1} 3.2% σ_{HOMO} 2.3% σ_{HOMO-7} 2.0% σ_{HOMO-6}
σ_{HOMO-4}	74.6% σ_{HOMO-5} 18.0% F_{2px}[b] 2.4% σ_{HOMO-8} 1.5% σ_{HOMO-7}	99.5% σ_{HOMO-4} 0.3% H_{4s}
σ_{HOMO-5}	47.2% σ_{HOMO-6} 22.3% F_{2pz}[c] 10.0% σ_{HOMO-7} 4.0% σ_{HOMO-1} 3.9% σ_{HOMO-4} 3.7% σ_{HOMO-2} 2.9% σ_{HOMO} 1.2% σ_{HOMO-3} 1.0% σ_{HOMO-9}	47.7% σ_{HOMO-5} 15.3% H_{1s} 7.6% σ_{HOMO-2} 6.4% σ_{HOMO-3} 6.4% σ_{HOMO-1} 5.9% σ_{HOMO-6} 4.7% σ_{HOMO-7} 1.0% σ_{HOMO-9}
σ_{HOMO-6}	51.2% σ_{HOMO-6} 20.9% F_{2pz}[c] 14.3% σ_{HOMO-7} 2.2% σ_{HOMO-8} 1.8% σ_{HOMO-1} 1.5% F_{2s} 1.5% σ_{HOMO-2} 1.4% σ_{HOMO}	90.2% σ_{HOMO-6} 3.5% σ_{HOMO-7} 3.0% H_{1s}

[a] Only contributions greater than 1% are listed. [b] doubly occupied orbital. [c] F_{2pz} corresponds to the SOMO of the fluorine.

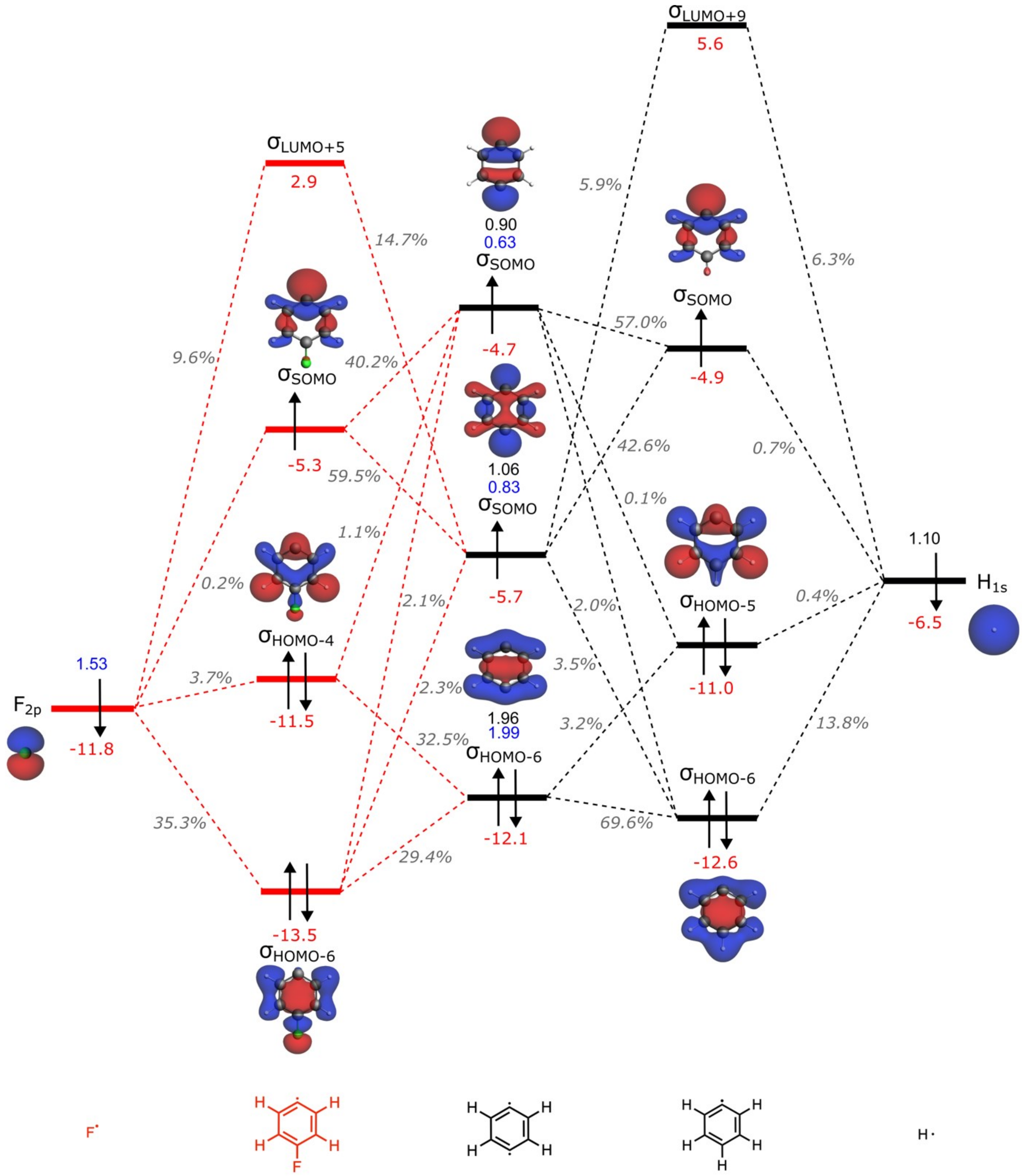

Figure S12. Qualitative MO diagram showing the formation of the σ_{SOMO} and $\sigma_{HOMO\text{-}6}$ of the *para*-aryl radical ($C_6H_4R^•$) from the interaction of $C_6H_4^{••}$ + $R^•$ (R = F *versus* H). The orbital energies (in eV) are given in red, gross population (in electrons) in blue (R = F) and black (R = H), and SFO Gross Mulliken contributions in gray. Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S6. SFO Gross Mulliken contributions (%)[a] to the MOs of the *para*-aryl radical ($C_6H_4R^{\bullet}$) formed from the interaction of $C_6H_4^{\bullet\bullet}$ + $R^{\bullet}$ (R = F or H). Computed at ZORA-BLYP-D3(BJ)/TZ2P.

MO	SFO Gross Mulliken contributions (%)	
	R =F	R = H
σ_{SOMO}	59.5% σ_{HOMO-1} 40.2% σ_{HOMO}	57.0% σ_{HOMO} 42.6% σ_{HOMO-1}
σ_{HOMO-1}	70.1% σ_{HOMO-2} 26.8% F_{2px}[b] 1.9% σ_{HOMO-4}	98.9% σ_{HOMO-1}
σ_{HOMO-2}	37.5% σ_{HOMO-5} 33.7% σ_{HOMO-6} 14.3% F_{2pz}[c] 5.8% σ_{HOMO-1} 5.3% σ_{HOMO} 1.4% σ_{HOMO-7}	27.8% H_{1s} 27.3% σ_{HOMO-2} 23.4% σ_{HOMO-6} 13.9% σ_{HOMO} 3.0% σ_{HOMO-5} 2.6% σ_{HOMO-7} 2.2% σ_{HOMO-9}
σ_{HOMO-3}	98.9% σ_{HOMO-3}	99.9% σ_{HOMO-3}
σ_{HOMO-4}	76.1% σ_{HOMO-4} 18.4% F_{2px}[b] 3.1% σ_{HOMO-8} 1.8% σ_{HOMO-2}	99.4% σ_{HOMO-4}
σ_{HOMO-5}	60.2% σ_{HOMO-5} 32.5% σ_{HOMO-6} 3.7% F_{2pz}[c] 1.1% σ_{HOMO} 1.1% σ_{HOMO-1}	95.9% σ_{HOMO-5} 3.2% σ_{HOMO-6}
σ_{HOMO-6}	35.3% F_{2pz}[c] 29.4% σ_{HOMO-6} 20.2% σ_{HOMO-7} 2.9% F_{2s} 2.6% σ_{HOMO-9} 2.3% σ_{HOMO-1} 2.1% σ_{HOMO} 1.5% σ_{HOMO-5}	69.6% σ_{HOMO-6} 13.8% H_{1s} 7.3% σ_{HOMO-7} 3.5% σ_{HOMO-1} 2.0% σ_{HOMO} 2.0% σ_{HOMO-9}

[a] Only contributions greater than 1% are listed. [b] doubly occupied orbital. [c] F_{2pz} corresponds to the SOMO of the fluorine.

Table S7. Energy decomposition analysis (in kcal mol^{-1}) of the *ortho*-C–H bond in *mono*-substituted benzenes C_6H_5R (R= H, F, Cl, Br, I, and Li) at a consistent geometry[a] with a C–H distance of 1.088 Å. Computed at ZORA-BLYP-D3(BJ)/TZ2P.

R	ΔH	ΔE	ΔE_{strain}	ΔE_{int}	ΔV_{elstat}	ΔE_{Pauli}	ΔE_{oi}	ΔE_{pb}	ΔE_{disp}	$\Delta E_{spinpol}$
H	–109.3	–115.9	1.8	–117.7	–64.9	94.9	–149.5	–96.5	–0.9	2.7
F	–111.8	–118.4	1.8	–120.2	–61.9	90.1	–150.2	–96.6	–1.0	2.8
Cl	–110.9	–117.5	1.9	–119.5	–63.0	93.0	–151.1	–98.4	–1.1	2.8
Br	–110.3	–117.0	2.0	–119.0	–63.2	95.8	–153.3	–100.2	–1.2	2.8
I	–109.4	–116.0	2.1	–118.1	–64.6	101.6	–156.8	–102.9	–1.2	3.0
Li	–91.9	–98.1	10.7	–108.9	–74.6	125.3	–161.1	–99.0	–1.0	2.6

[a] The equilibrium C–H bond length in benzene.

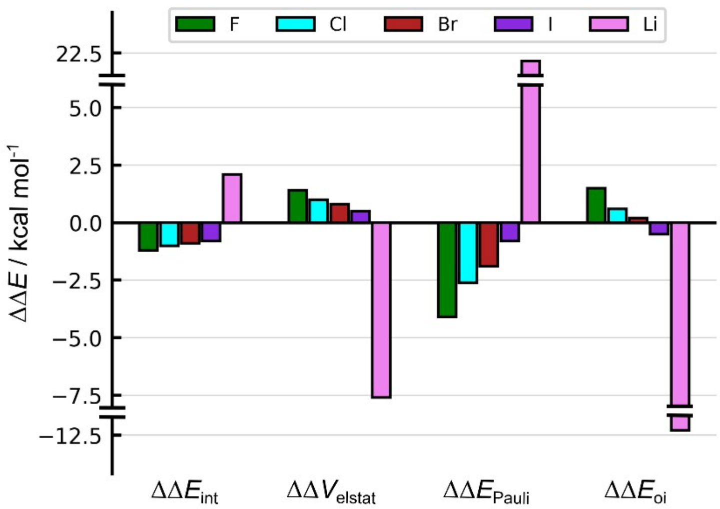

Figure S13. Energy decomposition analysis of the *para*-C–H bond in mono-substituted benzenes C_6RH_5 (R = F, Cl, Br, I, and Li) relative to benzene at a consistent geometry with a C–H distance of 1.088 Å. Computed at ZORA-BLYP-D3(BJ)/TZ2P.

Table S8. Cartesian coordinates (in Å), energies (electronic energy E and enthalpy H, in kcal mol^{-1}), number of imaginary frequencies (N_{imag}), and multiplicity (2S + 1) of all systems studied herein, computed at ZORA-BLYP-D3(BJ)/TZ2P.

C_6H_6 (B)
E = -1680.98
H = -1616.32
N_{imag} = 0
2S+1 = 1

C	-0.699921	1.212266	0.000000
C	0.000019	-0.000000	0.000000
C	-0.699921	-1.212266	0.000000
C	-2.099744	-1.212266	0.000000
C	-2.799685	-0.000000	0.000000
C	-2.099744	1.212266	0.000000
H	1.088024	-0.000000	0.000000
H	-0.155941	-2.154521	0.000000
H	-2.643725	-2.154521	0.000000
H	-3.887690	-0.000000	0.000000
H	-2.643725	2.154521	0.000000
H	-0.155941	2.154521	0.000000

C_6FH_5
E = -1686.67
H = -1626.62
N_{imag} = 0
2S+1 = 1

C	-0.705920	-1.211576	0.000000
C	-0.004809	-0.000002	0.000000
C	-0.705934	1.211563	0.000000
C	-2.105681	1.221204	0.000000
C	-2.773576	-0.000017	0.000000
C	-2.105667	-1.221232	-0.000000
H	1.082206	0.000007	0.000000
H	-0.165590	2.155299	0.000000
H	-2.672926	2.147805	0.000000
H	-2.672901	-2.147839	-0.000000
H	-0.165564	-2.155304	-0.000000
F	-4.146735	-0.000025	0.000000

1,2-$C_6F_2H_4$
E = -1687.79
H = -1632.25
N_{imag} = 0
2S + 1 = 1

C	-0.696861	1.222249	0.000000
C	-2.087865	1.220555	0.000000
C	-2.796240	0.015676	0.000000
C	-2.121220	-1.200588	0.000000
C	-0.721141	-1.204952	0.000000
C	-0.012134	0.001029	0.000000
F	-2.775566	2.397130	0.000000
F	-4.158751	0.044449	0.000000
H	-2.697448	-2.121902	0.000000

H	-0.189222	-2.152495	0.000000
H	-0.172049	2.173797	0.000000
H	1.074490	-0.002972	0.000000

1,3-$C_6F_2H_4$
E = -1691.54
H = -1636.1
N_{imag} = 0
2S+1 = 1

C	-0.714469	1.186415	0.000000
C	0.015198	-0.000000	0.000000
C	-0.714469	-1.186415	0.000000
C	-2.106607	-1.218461	0.000000
C	-2.795095	-0.000000	0.000000
C	-2.106607	1.218461	0.000000
H	1.100322	-0.000000	0.000000
F	-0.024542	-2.369034	0.000000
H	-2.626624	-2.171406	0.000000
H	-3.881956	-0.000000	0.000000
H	-2.626624	2.171406	0.000000
F	-0.024542	2.369034	0.000000

1,4-$C_6F_2H_4$
E = -1690.93
H = -1635.52
N_{imag} = 0
2S + 1 = 1

C	0.000000	1.220583	0.699724
C	0.000000	0.000000	1.369737
C	-0.000000	-1.220583	0.699724
C	-0.000000	-1.220583	-0.699724
C	-0.000000	0.000000	-1.369737
C	0.000000	1.220583	-0.699724
F	0.000000	0.000000	2.741728
H	0.000000	-2.148780	1.263656
H	0.000000	-2.148780	-1.263656
F	-0.000000	0.000000	-2.741728
H	-0.000000	2.148780	1.263656
H	-0.000000	2.148780	-1.263656

1,3,5-$C_6F_3H_3$
E = -1695.53
H = -1644.7
N_{imag} = 0
2S+1 = 1

C	-0.715204	1.185826	0.000000
C	0.015851	-0.000000	0.000000
C	-0.715204	-1.185826	0.000000
C	-2.107689	-1.226046	0.000000
C	-2.769133	-0.000000	0.000000
C	-2.107689	1.226046	0.000000
H	1.100327	-0.000000	0.000000
F	-0.032443	-2.368300	0.000000
H	-2.649899	-2.165247	0.000000

F	-4.134578	-0.000000	0.000000
H	-2.649899	2.165247	0.000000
F	-0.032443	2.368300	0.000000

1,2,3-$C_6F_3H_3$
E = -1688.34
H = -1637.27
N_{imag} = 0
2S+1 = 1

C	-0.696285	1.216849	0.000000
C	-0.005971	0.000000	0.000000
C	-0.696285	-1.216849	0.000000
C	-2.087933	-1.202596	0.000000
C	-2.800527	-0.000000	0.000000
C	-2.087933	1.202596	0.000000
H	1.080158	0.000000	0.000000
H	-0.178149	-2.171175	0.000000
F	-2.788389	-2.368960	0.000000
F	-4.154131	-0.000000	0.000000
F	-2.788390	2.368960	0.000000
H	-0.178149	2.171175	0.000000

1,2,4-$C_6F_3H_3$
E = -1691.47
H = -1640.55
N_{imag} = 0
2S + 1 = 1

C	-0.701434	1.197587	0.000000
C	0.001883	-0.002258	0.000000
C	-0.693970	-1.217131	0.000000
C	-2.085302	-1.186899	0.000000
C	-2.812850	0.001768	0.000000
C	-2.099802	1.197052	0.000000
H	1.087786	0.023501	0.000000
H	-0.170119	-2.167698	0.000000
F	-2.775539	-2.368653	0.000000
H	-3.898214	0.003246	0.000000
F	-2.767810	2.380854	0.000000
F	-0.035422	2.385818	0.000000

1,2,3,4-$C_6F_4H_2$
E = -1687.83
H = -1641.26
N_{imag} = 0
2S + 1 = 1

C	-0.703251	1.197175	0.000000
C	0.000786	-0.001626	0.000000
C	-0.699200	-1.213939	0.000000
C	-2.089402	-1.203595	0.000000
C	-2.800890	0.000642	0.000000
C	-2.101887	1.211258	0.000000
H	1.086093	0.021690	0.000000
H	-0.176773	-2.165526	0.000000

F	-2.789366	-2.369876	0.000000
F	-4.152405	0.004894	0.000000
F	-2.781296	2.379621	0.000000
F	-0.043203	2.386473	0.000000

1,2,4,5-$C_6F_4H_2$
E = -1690.93
H = -1644.52
$\boldsymbol{N_{imag}}$ = 0
2S+1 = 1

C	-0.701087	1.198327	0.000000
C	0.008042	-0.000000	0.000000
C	-0.701087	-1.198327	0.000000
C	-2.098580	-1.198327	0.000000
C	-2.807709	-0.000000	0.000000
C	-2.098580	1.198327	0.000000
H	1.093592	0.000000	0.000000
F	-0.030916	-2.380713	0.000000
F	-2.768751	-2.380713	0.000000
H	-3.893259	-0.000000	0.000000
F	-2.768751	2.380713	0.000000
F	-0.030916	2.380713	0.000000

1,2,3,5-$C_6F_4H_2$
E = -1691.23
H = -1644.79
$\boldsymbol{N_{imag}}$ = 0
2S + 1 = 1

C	-0.716229	1.183392	0.000000
C	0.012439	-0.003310	0.000000
C	-0.703474	-1.197870	0.000000
C	-2.101318	-1.215667	0.000000
C	-2.784863	0.003810	0.000000
C	-2.108277	1.221104	0.000000
H	1.097255	-0.005677	0.000000
F	-0.040172	-2.381877	0.000000
F	-2.778037	-2.387737	0.000000
F	-4.141896	-0.013836	0.000000
H	-2.652713	2.159416	0.000000
F	-0.033507	2.365825	0.000000

1,2,3,4,5-C_6F_5H
E = -1686.59
H = -1644.52
$\boldsymbol{N_{imag}}$ = 0
2S+1 = 1

C	-0.703448	1.196711	0.000000
C	0.007611	-0.000000	0.000000
C	-0.703448	-1.196711	0.000000
C	-2.100596	-1.213119	0.000000
C	-2.796925	-0.000000	0.000000
C	-2.100596	1.213119	0.000000
H	1.092728	0.000000	0.000000

F	-0.037856	-2.379615	0.000000
F	-2.781569	-2.380623	0.000000
F	-4.146470	-0.000000	0.000000
F	-2.781569	2.380623	0.000000
F	-0.037856	2.379615	0.000000

C_6ClH_5
E = -1644.02
H = -1584.52
N_{imag} = 0
2S+1 = 1

C	-0.000000	1.210060	0.755698
C	0.000000	-0.000000	1.458037
C	0.000000	-1.210060	0.755698
C	0.000000	-1.218540	-0.643299
C	0.000000	0.000000	-1.326354
C	-0.000000	1.218540	-0.643299
H	0.000000	-0.000000	2.545199
H	0.000000	-2.155285	1.293828
H	-0.000000	-2.152559	-1.197188
H	0.000000	2.152559	-1.197188
H	-0.000000	2.155285	1.293828
Cl	0.000000	-0.000000	-3.094961

C_6BrH_5
E = -1630.83
H = -1571.52
N_{imag} = 0
2S+1 = 1

C	-0.000000	1.210195	0.754897
C	0.000000	0.000000	1.456762
C	0.000000	-1.210195	0.754897
C	0.000000	-1.219194	-0.644925
C	0.000000	-0.000000	-1.324539
C	-0.000000	1.219194	-0.644925
H	0.000000	0.000000	2.543941
H	-0.000000	-2.155628	1.292792
H	-0.000000	-2.155029	-1.195293
H	0.000000	2.155029	-1.195293
H	0.000000	2.155628	1.292792
Br	0.000000	0.000000	-3.261108

C_6IH_5
E = -1617.95
H = -1558.76
N_{imag} = 0
2S+1 = 1

C	-0.000000	1.209810	0.755188
C	0.000000	0.000000	1.457273
C	0.000000	-1.209810	0.755188
C	0.000000	-1.218423	-0.644923
C	0.000000	-0.000000	-1.329964
C	-0.000000	1.218423	-0.644923
H	0.000000	0.000000	2.544526
H	-0.000000	-2.155659	1.292674

H	-0.000000	-2.158276	-1.188519
H	0.000000	2.158276	-1.188519
H	0.000000	2.155659	1.292674
I	0.000000	0.000000	-3.470675

C_6LiH_5
E = -1605.15
H = -1546.55
N_{imag} = 0
2S+1 = 1

C	-0.000000	1.206409	0.734846
C	0.000000	-0.000000	1.444272
C	0.000000	-1.206409	0.734846
C	0.000000	-1.193869	-0.668196
C	0.000000	0.000000	-1.435750
C	-0.000000	1.193869	-0.668196
H	0.000000	-0.000000	2.533123
H	0.000000	-2.153910	1.274768
H	-0.000000	-2.164958	-1.172433
H	0.000000	2.164958	-1.172433
H	-0.000000	2.153910	1.274768
Li	0.000000	-0.000000	-3.399617

$C_6H_5^{\cdot}$ ($B^{\cdot}$)
E = -1542.88
H = -1486.38
N_{imag} = 0
2S+1 = 2

C	-0.689910	1.227330	0.000000
C	-0.064741	-0.000000	0.000000
C	-0.689910	-1.227330	0.000000
C	-2.099806	-1.216435	0.000000
C	-2.792998	-0.000000	0.000000
C	-2.099806	1.216435	0.000000
H	-0.140402	2.166603	0.000000
H	-0.140402	-2.166603	0.000000
H	-2.643725	-2.159696	0.000000
H	-3.880579	-0.000000	0.000000
H	-2.643725	2.159696	0.000000

2-$C_6FH_4^{\cdot}$ (o)
E = -1546.14
H = -1494.12
N_{imag} = 0
2S+1 = 2

C	-0.705767	1.211096	0.000000
C	-0.055702	-0.000786	0.000000
C	-0.687207	-1.221261	0.000000
C	-2.098460	-1.214868	0.000000
C	-2.790741	0.001287	0.000000
C	-2.104652	1.222570	0.000000
F	-0.017255	2.392556	0.000000
H	-0.134615	-2.158913	0.000000
H	-2.638726	-2.158861	0.000000
H	-3.877830	0.003948	0.000000

H	-2.629055	2.176102	0.000000

3-$C_6FH_4^{\bullet}$ (m)
E = -1548.2
H = -1496.28
N_{imag} = 0
2S+1 = 2

C	-0.684033	1.233753	0.000000
C	-0.068485	0.001910	0.000000
C	-0.689185	-1.227588	0.000000
C	-2.098849	-1.212767	0.000000
C	-2.801332	-0.002559	0.000000
C	-2.085262	1.193571	0.000000
H	-0.155770	2.184183	0.000000
H	-0.140013	-2.165813	0.000000
H	-2.646118	-2.153705	0.000000
H	-3.886943	0.024140	0.000000
F	-2.776009	2.377744	0.000000

4-$C_6FH_4^{\bullet}$ (p)
E = -1547.3
H = -1495.38
N_{imag} = 0
2S+1 = 2

C	-0.691958	1.226989	0.000000
C	-0.064816	-0.000000	0.000000
C	-0.691958	-1.226989	0.000000
C	-2.100770	-1.225952	0.000000
C	-2.763665	-0.000000	0.000000
C	-2.100770	1.225952	0.000000
H	-0.143959	2.166615	0.000000
H	-0.143959	-2.166615	0.000000
H	-2.669716	-2.152315	0.000000
F	-4.136706	-0.000000	0.000000
H	-2.669716	2.152315	0.000000

2,3-$C_6F_2H_3^{\bullet}$ (o-m)
E = -1547.32
H = -1499.73
N_{imag} = 0
2S + 1 = 2

C	-0.671576	1.238402	0.000000
C	-2.076089	1.257212	0.000000
C	-2.806328	0.069970	0.000000
C	-2.136656	-1.158403	0.000000
C	-0.727181	-1.205499	0.000000
C	-0.072787	0.002992	0.000000
F	-2.720726	2.457524	0.000000
H	-3.891102	0.124460	0.000000
H	-2.704821	-2.085740	0.000000
H	-0.197999	-2.155374	0.000000
F	0.030047	2.402356	0.000000

3,4-$C_6F_2H_3^{\cdot}$ (m-p)
E = -1548.32
H = -1500.88
N_{imag} = 0
2S + 1 = 2

C	-0.666152	1.249336	0.000000
C	-2.066096	1.263415	0.000000
C	-2.789145	0.063953	0.000000
C	-2.141380	-1.167996	0.000000
C	-0.732720	-1.209623	0.000000
C	-0.079533	0.002364	0.000000
F	-2.739934	2.445497	0.000000
F	-4.151013	0.117344	0.000000
H	-2.735603	-2.078847	0.000000
H	-0.209612	-2.162401	0.000000
H	-0.113351	2.185892	0.000000

2,6-$C_6F_2H_3^{\cdot}$ (2o)
E = -1548.25
H = -1500.68
N_{imag} = 0
2S+1 = 2

C	-0.703042	1.208413	0.000000
C	-0.047226	-0.000000	0.000000
C	-0.703042	-1.208413	0.000000
C	-2.103242	-1.221420	0.000000
C	-2.787110	-0.000000	0.000000
C	-2.103242	1.221420	0.000000
F	-0.011377	2.383909	0.000000
F	-0.011377	-2.383909	0.000000
H	-2.625348	-2.175186	0.000000
H	-3.873660	-0.000000	0.000000
H	-2.625348	2.175186	0.000000

3,5-$C_6F_2H_3^{\cdot}$ (2m)
E = -1552.59
H = -1505.25
N_{imag} = 0
2S+1 = 2

C	-2.080103	1.192403	0.000000
C	-2.802453	0.000000	0.000000
C	-2.080103	-1.192403	0.000000
C	-0.678443	-1.234388	0.000000
C	-0.069492	0.000000	0.000000
C	-0.678443	1.234388	0.000000
H	-3.887123	0.000000	0.000000
F	-2.774174	-2.370870	0.000000
H	-0.148737	-2.183068	0.000000
F	-2.774174	2.370870	0.000000
H	-0.148737	2.183068	0.000000

2,4-$C_6F_2H_3^{\cdot}$ (o-p)
E = -1549.88
H = -1502.43

N_{imag} = 0
2S + 1 = 2

C	-0.684775	1.228080	0.000000
C	-2.082322	1.283078	0.000000
C	-2.771535	0.069665	0.000000
C	-2.139824	-1.172454	0.000000
C	-0.730379	-1.202975	0.000000
C	-0.064554	-0.000433	0.000000
H	-2.608566	2.233776	0.000000
F	-4.139910	0.109462	0.000000
H	-2.727463	-2.085879	0.000000
H	-0.203419	-2.154759	0.000000
F	0.029743	2.389761	0.000000

2,5-$C_6F_2H_3^{\cdot}$ (o-m')
E = -1550.08
H = -1502.65
N_{imag} = 0
2S + 1 = 2

C	-0.057530	-0.001771	0.000000
C	-0.705168	1.211522	0.000000
C	-2.103970	1.217284	0.000000
C	-2.798542	0.001518	0.000000
C	-2.082185	-1.193775	0.000000
C	-0.678939	-1.227354	0.000000
F	-0.018476	2.392643	0.000000
H	-2.633000	2.168071	0.000000
H	-3.883878	-0.023228	0.000000
F	-2.766354	-2.379604	0.000000
H	-0.147308	-2.176132	0.000000

2,3,4-$C_6F_3H_2^{\cdot}$ (o-m-p)
E = -1546.98
H = -1503.89
N_{imag} = 0
2S + 1 = 2

C	-0.069154	0.000192	0.000000
C	-0.729768	-1.204141	0.000000
C	-2.138714	-1.165434	0.000000
C	-2.782536	0.068756	0.000000
C	-2.069787	1.275380	0.000000
C	-0.666782	1.237340	0.000000
H	-0.204932	-2.156215	0.000000
H	-2.730852	-2.076623	0.000000
F	-4.141677	0.128774	0.000000
F	-2.726389	2.458672	0.000000
F	0.034939	2.398709	0.000000

2,3,6-$C_6F_3H_2^{\cdot}$ (2o-m)
E = -1548.25
H = -1505.15
N_{imag} = 0

2S + 1 = 2

C	-2.062034	1.203554	0.000000
C	-2.759859	-0.001403	0.000000
C	-2.066552	-1.217912	0.000000
C	-0.667798	-1.209782	0.000000
C	-0.017917	0.002267	0.000000
C	-0.655588	1.218087	0.000000
H	-3.845383	0.021922	0.000000
H	-2.593410	-2.169140	0.000000
F	0.024448	-2.383890	0.000000
F	0.017263	2.395027	0.000000
F	-2.731972	2.388458	0.000000

2,3,5-$C_6F_3H_2^{\bullet}$ (o-2m)
E = -1550.48
H = -1507.50
Nimag = 0
2S + 1 = 2

C	-0.693898	1.222568	0.000000
C	-0.069798	0.000244	0.000000
C	-0.683172	-1.229350	0.000000
C	-2.085455	-1.191508	0.000000
C	-2.805980	0.001848	0.000000
C	-2.098728	1.203216	0.000000
H	-0.149856	-2.176343	0.000000
F	-2.775543	-2.370885	0.000000
H	-3.890921	0.002776	0.000000
F	-2.776379	2.381958	0.000000
F	-0.021390	2.402662	0.000000

2,3,5-$C_6F_3H_2^{\bullet}$ (o-m-p')
E = -1549.73
H = -1506.78
N_{imag} = 0
2S + 1 = 2

C	-2.052704	1.209871	0.000000
C	-0.651649	1.225065	0.000000
C	-0.024704	0.001115	0.000000
C	-0.671287	-1.212251	0.000000
C	-2.070560	-1.226997	0.000000
C	-2.744965	-0.007198	0.000000
H	-0.120373	2.174234	0.000000
F	0.012396	-2.391666	0.000000
H	-2.622482	-2.163595	0.000000
F	-4.104255	0.007214	0.000000
F	-2.751122	2.376192	0.000000

2,4,6-$C_6F_3H_2^{\bullet}$ (2o-p)
E = -1551.31
H = -1508.32
N_{imag} = 0
2S+1 = 2

C	-0.704533	1.207798	0.000000
C	-0.046381	-0.000000	0.000000
C	-0.704533	-1.207798	0.000000
C	-2.104029	-1.230281	0.000000
C	-2.761276	-0.000000	0.000000
C	-2.104029	1.230281	0.000000
F	-0.016739	2.381805	0.000000
F	-0.016739	-2.381805	0.000000
H	-2.650605	-2.168658	0.000000
F	-4.126538	-0.000000	0.000000
H	-2.650605	2.168658	0.000000

3,4,5-$C_6F_3H_2^{\cdot}$ (2m-p)
E = -1548.66
H = -1505.69
N_{imag} = 0
2S+1 = 2

C	-0.686462	1.233694	0.000000
C	-0.076491	0.000000	0.000000
C	-0.686462	-1.233694	0.000000
C	-2.087114	-1.209227	0.000000
C	-2.792170	0.000000	0.000000
C	-2.087114	1.209227	0.000000
H	-0.156292	-2.182522	0.000000
F	-2.794331	-2.369750	0.000000
F	-4.146146	0.000000	0.000000
F	-2.794331	2.369750	0.000000
H	-0.156292	2.182522	0.000000

2,3,4,5-$C_6F_4H^{\cdot}$ (o-2m-p)
E = -1546.22
H = -1507.60
N_{imag} = 0
2S + 1 = 2

C	-0.696275	1.222661	0.000000
C	-0.072296	0.000725	0.000000
C	-0.688736	-1.227259	0.000000
C	-2.089395	-1.209055	0.000000
C	-2.793222	0.000871	0.000000
C	-2.100628	1.218429	0.000000
H	-0.154731	-2.174307	0.000000
F	-2.791959	-2.371302	0.000000
F	-4.145042	0.004313	0.000000
F	-2.792404	2.379847	0.000000
F	-0.026432	2.402265	0.000000

2,3,5,6-$C_6F_4H^{\cdot}$ (2o-2m)
E = -1547.48
H = -1508.83
N_{imag} = 0
2S+1 = 2

C	-0.690326	1.220452	0.000000
C	-0.060869	0.000000	0.000000
C	-0.690326	-1.220452	0.000000

C	-2.095363	-1.202694	0.000000
C	-2.799473	-0.000000	0.000000
C	-2.095363	1.202694	0.000000
F	-0.014276	2.394982	0.000000
F	-0.014276	-2.394982	0.000000
F	-2.770509	-2.382096	0.000000
H	-3.884714	-0.000000	0.000000
F	-2.770509	2.382096	0.000000

2,3,4,6-$C_6F_4H^{\cdot}$ (2o-m-p)
E = -1547.28
H = -1508.65
$\boldsymbol{N_{imag}}$ = 0
2S + 1 = 2

C	-0.705513	1.206011	0.000000
C	-0.054393	-0.004414	0.000000
C	-0.695008	-1.219800	0.000000
C	-2.099944	-1.222453	0.000000
C	-2.777712	0.002834	0.000000
C	-2.104468	1.223432	0.000000
F	-0.024183	-2.395738	0.000000
F	-2.783807	-2.389303	0.000000
F	-4.134786	-0.013648	0.000000
H	-2.653698	2.161059	0.000000
F	-0.017607	2.379594	0.000000

$C_6F_5^{\cdot}$ (2o-2m-p)
E = -1542.68
H = -1508.37
$\boldsymbol{N_{imag}}$ = 0
2S+1 = 2

C	-0.693078	1.219396	0.000000
C	-0.062661	-0.000000	0.000000
C	-0.693078	-1.219396	0.000000
C	-2.097271	-1.218447	0.000000
C	-2.787785	-0.000000	0.000000
C	-2.097271	1.218447	0.000000
F	-0.019080	2.393408	0.000000
F	-0.019080	-2.393408	0.000000
F	-2.785519	-2.381454	0.000000
F	-4.137652	-0.000000	0.000000
F	-2.785519	2.381454	0.000000

$C_6ClH_4^{\cdot}$ (o-Cl)
E = -1504.33
H = -1452.91
$\boldsymbol{N_{imag}}$ = 0
2S+1 = 2

C	-0.730164	1.204374	0.000000
C	-2.139648	1.159802	0.000000
C	-2.798945	-0.075210	0.000000
C	-2.082525	-1.277660	0.000000
C	-0.678135	-1.236031	0.000000
C	-0.073514	-0.003716	0.000000

H	-2.706457	2.088447	0.000000
H	-3.885775	-0.107366	0.000000
H	-2.591525	-2.238719	0.000000
H	-0.199874	2.154607	0.000000
Cl	0.266570	-2.728627	0.000000

$C_6BrH_4^{\cdot}$ (o-Br)
E = -1491.73
H = -1440.52
N_{imag} = 0
2S+1 = 2

C	-0.728178	1.203447	0.000000
C	-2.137616	1.158376	0.000000
C	-2.799360	-0.075703	0.000000
C	-2.085796	-1.280824	0.000000
C	-0.682617	-1.233205	0.000000
C	-0.075881	-0.008224	0.000000
H	-2.704049	2.087331	0.000000
H	-3.886327	-0.105708	0.000000
H	-2.598283	-2.239692	0.000000
H	-0.197002	2.153049	0.000000
Br	0.363876	-2.863935	0.000000

$C_6IH_4^{\cdot}$ (o-I)
E = -1479.82
H = -1428.75
N_{imag} = 0
2S+1 = 2

C	-0.727347	1.202258	0.000000
C	-2.136535	1.158482	0.000000
C	-2.801017	-0.074538	0.000000
C	-2.090652	-1.281844	0.000000
C	-0.685208	-1.235624	0.000000
C	-0.080319	-0.013442	0.000000
H	-2.702074	2.088152	0.000000
H	-3.888230	-0.101859	0.000000
H	-2.609826	-2.237130	0.000000
H	-0.194187	2.150661	0.000000
I	0.488583	-3.030780	0.000000

$C_6LiH_4^{\cdot}$ (o-Li)
E = -1484.86
H = -1433.94
N_{imag} = 0
2S+1 = 2

C	-0.649668	0.956262	0.000000
C	-2.049350	1.066943	0.000000
C	-2.868818	-0.077598	0.000000
C	-2.312955	-1.366947	0.000000
C	-0.909725	-1.436929	0.000000
C	-0.131009	-0.349503	0.000000
H	-2.509945	2.054689	0.000000
H	-3.952314	0.040171	0.000000
H	-2.957673	-2.245259	0.000000
H	-0.026024	1.849677	0.000000

Li	1.018988	-1.995100	0.000000

$C_6H_4^{\cdot\cdot}$ (o)
E = -1370.15
2S+1 = 3

C	-0.6999215	1.2122656	0.0000000
C	0.0000193	-0.0000000	0.0000000
C	-0.6999215	-1.2122656	0.0000000
C	-2.0997443	-1.2122656	0.0000000
C	-2.7996851	-0.0000000	0.0000000
C	-2.0997443	1.2122656	0.0000000
H	-2.6437248	-2.1545211	0.0000000
H	-3.8876897	-0.0000000	0.0000000
H	-2.6437248	2.1545211	0.0000000
H	-0.1559410	2.1545212	0.0000000

$C_6H_4^{\cdot\cdot}$ (m)
E = -1372.57
2S+1 = 3

C	-0.6999215	1.2122656	0.0000000
C	0.0000194	-0.0000000	0.0000000
C	-0.6999215	-1.2122656	0.0000000
C	-2.0997443	-1.2122656	0.0000000
C	-2.7996852	-0.0000000	0.0000000
C	-2.0997443	1.2122656	0.0000000
H	-0.1559410	-2.1545211	0.0000000
H	-3.8876897	-0.0000000	0.0000000
H	-2.6437248	2.1545211	0.0000000
H	-0.1559410	2.1545211	0.0000000

$C_6H_4^{\cdot\cdot}$ (p)
E = -1372.21
2S+1 = 3

C	-0.6999215	1.2122656	0.0000000
C	0.0000194	-0.0000000	0.0000000
C	-0.6999215	-1.2122656	0.0000000
C	-2.0997443	-1.2122656	0.0000000
C	-2.7996852	-0.0000000	0.0000000
C	-2.0997443	1.2122656	0.0000000
H	-0.1559410	-2.1545211	0.0000000
H	-2.6437248	-2.1545211	0.0000000
H	-2.6437248	2.1545211	0.0000000
H	-0.1559410	2.1545211	0.0000000