Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Electronic structures and optical properties of the IPR-violating $C_{60}X_8$ (X=H, F, and Cl) fullerene compounds: A computational study

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Table S1. Pyramidalization angles (degree) of the sp^2 carbon atoms in C_{60} (C_{2v}) and $C_{60}X_8$ (X=H, F, and Cl).

Carbon atoms	Pyramidalization angle (deg.)			
	C_{60} (C_{2v})	$C_{60}H_8$	$C_{60}F_8$	$C_{60}Cl_8$
1, 5, 8, 9	12.35	8.43	8.60	8.30
2, 6, 36, 42	11.42	9.17	9.17	9.14
3, 7, 21, 22	8.67	4.78	4.70	4.98
4, 17, 46, 50	12.91	9.49	9.74	9.42
10, 19, 30, 55	10.90			
11, 15, 18, 25	11.69	10.21	10.35	10.39
12, 24	12.44	10.71	10.89	10.98
13, 16, 40, 47	14.88			
14, 20, 29, 44	11.14	8.66	8.58	8.57
23, 35, 37, 49	11.74	10.35	10.51	10.58
26, 28	11.28	11.88	11.83	11.83
27, 39	10.93	9.88	10.07	10.02
31, 33, 34, 53	11.79	12.42	12.31	12.36
32, 38, 41, 54	11.67	11.76	11.76	11.76
43, 51, 58, 60	11.57	11.74	11.73	11.74
45, 48, 52, 56	11.76	12.07	12.00	12.04
57, 59	11.66	11.88	11.84	11.74

Table S2. The NICS values at all pentagon and hexagon ring centers, as well as values 1.0 Å above [NICS(1)] and below [NICS(-1)] each ring of two separate conjugated annulene subunits in $C_{60}X_8$ (X=H, F and Cl).

NICS(ppm)	A'	A	B	C	D	E	F
C_{60} (C_{2v})	4.7(1)	0.0 (1)	4.3(1)	-0.3(1)	0.4(1)	7.2(1)	0.3(1)
	7.2(0)	-1.8(0)	7.6(0)	-2.3(0)	-1.6(0)	13.8(0)	0.0(0)
	3.4(-1)	-3.2(-1)	3.4(-1)	-4.4(-1)	-3.8(-1)	4.6(-1)	-2.3(-1)
$C_{60}H_8$	-6.6(1)	-4.4(1)	1.5(1)	-1.9(1)	-2.2(1)	3.4(1)	-4.5(1)
	-10.9(0)	-11.0(0)	1.6(0)	-7.8(0)	-8.5(0)	4.7(0)	-11.3(0)
	-18.5(-1)	-19.4(-1)	-13.5(-1)	-19.3(-1)	-19.9(-1)	-12.5(-1)	-19.8(-1)
$C_{60}F_8$	-6.2(1)	-4.3(1)	1.2(1)	-2.0(1)	-2.3(1)	3.1(1)	-4.2(1)
	-11.5(0)	-11.2(0)	0.9(0)	-8.2(0)	-8.8(0)	3.8(0)	-11.2(0)
	-18.8(-1)	-20.0(-1)	-14.4(-1)	-20.0(-1)	-20.8(-1)	-13.5(-1)	-20.2(-1)
$C_{60}Cl_8$	-6.3(1)	-4.7(1)	1.2(1)	-2.1(1)	-2.4(1)	3.1(1)	-4.4(1)
	-11.7(0)	-11.5(0)	0.9(0)	-8.2(0)	-8.8(0)	3.9(0)	-11.4(0)
	-18.3(-1)	-19.8(-1)	-14.2(-1)	-19.8(-1)	-20.5(-1)	-13.2(-1)	-20.2(0)

Table S3. TD-DFT (B3LYP) calculated excitation energies (ΔE), oscillator strengths (f_{osc}), the largest coefficients in the configurational interaction (CI) expansions, and major transition composition with f_{osc}>0.100 of C_{60} (C_{2v}) and $C_{60}X_8$ compounds, in which the H and L refer to HOMO and LUMO.

State	Sym.	ΔE(eV)(nm)	f_{osc}	CI coefficient	Major configuration
			C_{2v}-C_{60}		
E_{111}	B_1	4.83 (256.9)	0.1351	0.43075	H-3→L+12 (37%)
E_{124}	A_1	5.01 (247.0)	0.4420	0.40117	H-1→L+12 (32%)
E_{135}	B_2	4.94 (238.2)	0.2697	0.43524	H-6→L+5 (38%)
E_{166}	B_2	5.52 (224.6)	0.1166	0.45624	H-5→L+12 (42%)
E_{225}	B_2	5.95 (208.0)	0.1340	0.43857	H→L+17 (38%)
E_{231}	B_2	6.00 (206.5)	0.3340	0.35888	H→L+17 (26%)
E_{233}	A_1	6.01 (206.2)	0.1483	0.26012	H-12→L+11 (14%)
E_{234}	B_2	5.56 (205.7)	0.1513	0.36306	H-14→L+3 (26%)
E_{236}	B_1	5.58 (205.4)	0.3975	0.42218	H-11→L+10 (36%)
E_{238}	B_2	6.06 (204.4)	0.1096	0.29097	H-7→L+11 (17%)
E_{242}	A_1	6.09 (203.3)	0.2043	0.36966	H-12→L+11 (27%)
E_{256}	B_2	6.23 (198.9)	0.1102	0.43649	H-28→L+2 (38%)
E_{270}	B_1	6.34 (195.5)	0.1749	0.37469	H-1→L+18 (28%)
E_{276}	B_1	6.37 (194.5)	0.1115	0.44636	H-21→L+3 (40%)
E_{301}	A_1	6.57 (188.6)	0.1592	0.37134	H-2→L+20 (28%)
			$C_{60}H_8$		
E_{102}	B_1	5.14 (241.0)	0.1334	0.48403	H-6→L+6 (47%)
E_{109}	B_1	5.27 (235.4)	0.2723	0.44830	H-6→L+6 (40%)
E_{164}	B_1	5.90 (209.3)	0.1008	0.48999	H-22→L+1 (28%)
E_{173}	B_1	5.98 (207.4)	0.2419	0.37129	H-22->L+1 (28%)
E_{214}	A_1	6.39 (194.1)	0.1126	0.46351	H-18→L+2 (43%)
E_{215}	B_1	6.42 (193.1)	0.1235	0.52194	H-8→L+13 (54%)
E_{233}	A_1	6.56 (189.1)	0.1663	0.50269	H→L+17 (51%)
E_{257}	B_2	6.79 (182.7)	0.1525	0.36155	H-2→L+16 (26%)
E_{300}	A_1	7.12 (174.2)	0.1119	0.47861	H-14→L+7 (46%)

			$C_{60}F_8$		
E_{71}	B_2	4.58 (270.4)	0.2025	0.37786	H→L+9 (29%)
E_{78}	B_1	4.69 (264.2)	0.1029	0.49619	H→L+10 (49%)
E_{100}	A_1	5.02 (246.6)	0.1017	0.31622	H-1→L+10 (20%)
E_{131}	B_1	5.35 (231.4)	0.1227	0.42332	H-11→L+3 (36%)
E_{205}	B_1	5.98 (207.3)	0.3078	0.03938	H-6→L+12 (28%)
E_{241}	A_1	6.24 (198.7)	0.2395	0.29274	H-9→L+8 (17%)
E_{254}	B_1	6.35 (195.1)	0.2399	0.51345	H-8→L+13 (53%)
E_{278}	A_1	6.51 (190.5)	0.1069	0.56749	H-10→L+11 (64%)
E_{302}	A_1	6.68 (185.6)	0.1002	0.52113	H-26→L+4 (54%)
			$C_{60}Cl_8$		
E_{89}	B_2	4.57 (271.0)	0.1330	0.59724	H-9→L+3 (71%)
E_{170}	B_1	5.14 (241.1)	0.1576	0.37613	H-4→L+10 (28%)
E_{184}	B_2	5.23 (236.8)	0.1084	0.49039	H-10→L+6 (48%)
E_{242}	A_1	5.61 (220.6)	0.1349	0.27969	H-29→L+1 (29%)
E_{264}	B_1	5.78 (214.5)	0.1618	0.36658	H-6→L+12 (27%)
E_{265}	B_2	5.78 (214.3)	0.1059	0.39574	H-29→L+2 (31%)
E_{275}	B_2	5.84 (212.3)	0.1145	0.35545	H-31→L+1 (25%)
E_{280}	B_1	5.86 (211.4)	0.1011	0.39401	H-35→L (31%)
E_{332}	B_1	6.19 (200.3)	0.1350	0.36680	H-8→L+13 (27%)
E_{335}	B_2	6.20 (200.1)	0.1453	0.37301	H-38→L (28%)