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Supporting Information

Structural and Spectral Properties of Non-classical C_{58} Isomer and its Fluorinated Derivatives in Theory

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Atoms	Coordinates		
	X	Y	Z
C	1.428110	2.186159	-2.255140
C	0.726879	3.079880	-1.440888
C	-0.726879	3.079880	-1.440888
C	-1.170746	3.322061	-0.083449
C	-2.358010	2.733351	0.373052
C	-2.386950	2.221883	1.698364
C	-3.117682	0.956218	1.698364
C	-2.413392	0.020454	2.470042
C	-2.339555	-1.350743	2.042247
C	-1.188982	-2.100286	2.470042
C	-0.730732	-3.178101	1.698364
C	0.730732	-3.178101	1.698364
C	1.188147	-3.408772	0.373052
C	2.291616	-2.674926	-0.083449
C	2.303814	-2.169436	-1.440888
C	3.030694	-0.910444	-1.440888
C	2.607324	0.143700	-2.255140
C	2.619835	1.512563	-1.752366
C	0.700712	1.242034	-3.079548
C	1.425989	-0.014182	-3.079548
C	0.725277	-1.227851	-3.079548
C	1.179214	-2.329859	-2.255140
C	0.000000	-3.025125	-1.752366
C	0.000000	-3.568321	-0.474773

C	-1.188147	-3.408772	0.373052
C	-2.291616	-2.674926	-0.083449
C	-2.926732	-1.689749	0.776371
C	-3.462362	-0.647134	-0.083449
C	-3.546156	0.675421	0.373052
C	-3.090257	1.784161	-0.474773
C	-2.619835	1.512563	-1.752366
C	-1.428110	2.186159	-2.255140
C	-0.700712	1.242034	-3.079548
C	-1.425989	-0.014182	-3.079548
C	-0.725277	-1.227851	-3.079548
C	-1.179214	-2.329859	-2.255140
C	-2.303814	-2.169436	-1.440888
C	-3.030694	-0.910444	-1.440888
C	-2.607324	0.143700	-2.255140
C	1.170746	3.322061	-0.083449
C	0.000000	3.379499	0.776371
C	0.000000	2.701485	2.042247
C	-1.224410	2.079832	2.470042
C	-1.226151	0.707919	2.983248
C	0.000000	0.000000	3.181209
C	0.000000	-1.415837	2.983248
C	1.188982	-2.100286	2.470042
C	2.339555	-1.350743	2.042247
C	2.926732	-1.689749	0.776371
C	3.462362	-0.647134	-0.083449
C	3.546156	0.675421	0.373052
C	3.090257	1.784161	-0.474773
C	2.358010	2.733351	0.373052

C	2.386950	2.221883	1.698364
C	1.224410	2.079832	2.470042
C	1.226151	0.707919	2.983248
C	2.413392	0.020454	2.470042
C	3.117682	0.956218	1.698364

2. Optimized coordinates of the singlet C_2-$^{\#1078}C_{58}$ in gas phase:

Table S2. Coordinates of optimized structure of the singlet C_2-$^{\#1078}C_{58}$ in gas phase at the B3LYP/6-311++G (3*df*, 3*pd*)//B3LYP/6-31G** level.

Atoms	Coordinates		
	X	Y	Z
C	2.864184	-0.909983	-1.027347
C	2.498273	0.271123	-1.716993
C	2.619165	1.568678	-1.014754
C	1.905539	2.704756	-1.527649
C	1.323571	3.644704	-0.646759
C	-0.063912	3.900824	-1.081369
C	-0.936992	3.738598	0.050094
C	-2.088541	2.946616	-0.109264
C	-2.534529	2.102758	0.976812
C	-3.098026	0.887550	0.407637
C	-3.040901	-0.306040	1.102814
C	-2.853388	-1.553882	0.394469
C	-2.138036	-2.447625	1.282485
C	-1.301566	-3.436841	0.753114
C	0.089767	-3.538018	1.222479
C	0.936992	-3.738598	0.050094
C	2.088541	-2.946616	-0.109264
C	2.313317	-2.210479	-1.357171
C	3.098026	-0.887550	0.407637

C	2.534529	-2.102758	0.976812
C	1.793915	-2.021857	2.161044
C	0.515869	-2.710659	2.256318
C	-0.415332	-1.814583	2.929626
C	-1.722531	-1.684067	2.446230
C	-2.335861	-0.376242	2.371970
C	-1.674275	0.751401	2.855620
C	-1.793915	2.021857	2.161044
C	-0.515869	2.710659	2.256318
C	-0.089767	3.538018	1.222479
C	1.301566	3.436841	0.753114
C	2.138036	2.447625	1.282485
C	2.853388	1.553882	0.394469
C	3.040901	0.306040	1.102814
C	2.335861	0.376242	2.371970
C	1.674275	-0.751401	2.855620
C	0.312125	-0.626177	3.340189
C	-0.312125	0.626177	3.340189
C	0.415332	1.814583	2.929626
C	1.722531	1.684067	2.446230
C	0.936992	2.519831	-2.610629
C	-0.290815	3.247731	-2.272930
C	-1.39200	2.331233	-2.403410
C	-2.313317	2.210479	-1.357171
C	-2.864184	0.909983	-1.027347
C	-2.498273	-0.271123	-1.716993
C	-2.619165	-1.568678	-1.014754
C	-1.905539	-2.704756	-1.527649
C	-1.323571	-3.644704	-0.646759

C	0.063912	-3.900824	-1.081369
C	0.290815	-3.247731	-2.272930
C	1.392000	-2.331233	-2.403410
C	0.881831	-1.119406	-2.993371
C	1.455079	0.127335	-2.746759
C	0.603162	1.259070	-3.042496
C	-0.881831	1.119406	-2.993371
C	-1.455079	-0.127335	-2.746759
C	-0.603162	-1.259070	-3.042496
C	-0.936992	-2.519831	-2.610629

3. Optimized coordinates of the singlet C_s-C_{58} (NC) in gas phase:

Table S3. Coordinates of optimized structure of the singlet C_s-C_{58} (NC) in gas phase at the B3LYP/6-311++G (3*df*, 3*pd*)//B3LYP/6-31G** level.

Atoms	Coordinates		
	X	Y	Z
C	2.476850	-2.112987	0.000000
C	2.899650	-1.354333	1.159976
C	2.219572	-1.494842	2.366021
C	1.174463	-2.445909	2.439654
C	0.560003	-2.996499	1.283382
C	1.237699	-2.870105	0.000000
C	2.89965	-1.354333	-1.159976
C	3.338378	-0.049116	-0.724574
C	3.338378	-0.049116	0.724574
C	2.942073	1.090481	1.434019
C	1.823687	-0.305320	3.141951
C	0.156999	-1.903661	3.337379
C	-1.081319	-2.223031	2.833366
C	-0.898456	-2.908777	1.543314

C	0.560003	-2.996499	-1.283382
C	1.174463	-2.445909	-2.439654
C	2.219572	-1.494842	-2.366021
C	2.942073	1.090481	-1.434019
C	2.138902	0.953423	-2.641079
C	1.823687	-0.305320	-3.141951
C	0.501589	-0.558514	-3.701099
C	0.156999	-1.903661	-3.337379
C	-1.081319	-2.223031	-2.833366
C	-0.898456	-2.908777	-1.543314
C	-1.953970	-2.501872	-0.713120
C	-1.953970	-2.501872	0.713120
C	0.501589	-0.558514	3.701099
C	-3.075852	0.961058	1.184258
C	-2.319086	1.196321	2.335048
C	-1.304342	2.233680	2.324524
C	-1.106899	3.002047	1.177097
C	-1.933186	2.795486	0.000000
C	-3.075852	0.961058	-1.184258
C	-3.281261	-0.404292	-0.729385
C	-3.281261	-0.404292	0.729385
C	-2.742403	-1.464094	1.433560
C	-2.102848	-1.231158	2.710297
C	-1.831965	0.082224	3.135771
C	-0.164337	1.740606	3.085255
C	1.129213	2.004475	2.629262
C	1.334384	2.800458	1.428248
C	0.240240	3.308062	0.725421
C	0.240240	3.308062	-0.725421

C	-1.106899	3.002047	-1.177097
C	-1.304342	2.233680	-2.324524
C	-2.319086	1.196321	-2.335048
C	-2.742403	-1.464094	-1.433560
C	-2.102848	-1.231158	-2.710297
C	-1.831965	0.082224	-3.135771
C	-0.498693	0.427856	-3.616409
C	-0.164337	1.740606	-3.085255
C	1.129213	2.004475	-2.629262
C	1.334384	2.800458	-1.428248
C	2.460413	2.241686	-0.702016
C	2.460413	2.241686	0.702016
C	-0.498693	0.427856	3.616409
C	2.138902	0.953423	2.641079
C	-2.897631	1.785689	0.000000

4. Optimized coordinates of C_s-C_{58}(NC)F_{18}(A) in gas phase:

Table S4. Coordinates of optimized structure of C_s-C_{58}(NC)F_{18}(A) in gas phase at the B3LYP/6-311++G (3*df*, 3*pd*)//B3LYP/6-31G** level.

Atoms	Coordinates		
	X	Y	Z
C	3.514085	-0.064726	0.000000
C	3.204524	0.851187	1.176880
C	2.641587	0.445607	2.353679
C	2.332781	-0.992752	2.671684
C	1.864024	-1.767883	1.371830
C	2.675390	-1.451171	0.000000
C	3.204524	0.851187	-1.176880
C	3.021304	2.196967	-0.720495
C	3.021304	2.196967	0.720495

C	2.230321	3.105575	1.425692
C	1.770708	1.338888	3.062731
C	1.058005	-0.901711	3.645416
C	-0.042403	-1.732462	2.964940
C	0.361612	-1.644557	1.516572
C	1.864024	-1.767883	-1.371830
C	2.332781	-0.992752	-2.671684
C	2.641587	0.445607	-2.353679
C	2.230321	3.105575	-1.425692
C	1.562130	2.645594	-2.610880
C	1.770708	1.338888	-3.062731
C	0.698954	0.564269	-3.622365
C	1.058005	-0.901711	-3.645416
C	-0.042403	-1.732462	-2.964940
C	0.361612	-1.644557	-1.516572
C	-0.702706	-1.576350	-0.714362
C	-0.702706	-1.57635	0.714362
C	0.698954	0.564269	3.622365
C	-3.148797	0.496516	1.169666
C	-2.567253	1.005041	2.299823
C	-2.054790	2.349460	2.279295
C	-2.214340	3.177298	1.167666
C	-2.863387	2.646453	0.000000
C	-3.148797	0.496516	-1.169666
C	-3.188692	-0.970265	-0.814492
C	-3.188692	-0.970265	0.814492
C	-1.998867	-1.708465	1.483946
C	-1.567387	-1.312607	2.963917
C	-1.838904	0.191718	3.369232

C	-0.817875	2.365401	3.025321
C	0.228833	3.190228	2.609172
C	0.082829	4.026480	1.428065
C	-1.127312	4.033640	0.723370
C	-1.127312	4.033640	-0.723370
C	-2.214340	3.177298	-1.167666
C	-2.054790	2.349460	-2.279295
C	-2.567253	1.005041	-2.299823
C	-1.998867	-1.708465	-1.483946
C	-1.567387	-1.312607	-2.963917
C	-1.838904	0.191718	-3.369232
C	-0.580709	1.045785	-3.550556
C	-0.817875	2.365401	-3.025321
C	0.228833	3.190228	-2.609172
C	0.082829	4.026480	-1.428065
C	1.331853	3.988272	-0.700141
C	1.331853	3.988272	0.700141
C	-0.580709	1.045785	3.550556
C	1.562130	2.645594	2.610880
C	-3.275110	1.311299	0.000000
F	-4.351259	-1.562131	1.246909
F	-4.351259	-1.562131	-1.246909
F	-2.328008	-3.052022	1.501950
F	-2.328008	-3.052022	-1.501950
F	-2.249922	-2.102654	-3.839052
F	-2.249922	-2.102654	3.839052
F	-2.578643	0.178178	4.543164
F	-2.578643	0.178178	-4.543164
F	0.039703	-3.027930	3.425857

F	0.039703	-3.027930	-3.425857
F	1.361229	-1.356724	-4.899806
F	1.361229	-1.356724	4.899806
F	2.096203	-3.113464	1.613171
F	2.096203	-3.113464	-1.613171
F	3.375202	-1.647323	3.264946
F	3.375202	-1.647323	-3.264946
F	3.660292	-2.403600	0.000000
F	4.857476	-0.403997	0.000000

5. Optimized coordinates of C_s-C_{58}(NC)F_{18}(B) in gas phase:

Table S5. Coordinates of optimized structure of C_s-C_{58}(NC)F_{18}(B) in gas phase at the B3LYP/6-311++G (3*df*, 3*pd*)//B3LYP/6-31G** level. in gas phase.

Atoms	Coordinates		
	X	Y	Z
C	-1.361201	2.885628	0.000000
C	-2.163269	2.512080	1.183744
C	-1.547166	2.257829	2.387651
C	-0.126368	2.689344	2.651726
C	0.75663	2.650165	1.322312
C	-0.004188	2.800079	0.000000
C	-2.163269	2.512080	-1.183744
C	-3.263325	1.712664	-0.734468
C	-3.263325	1.712664	0.734468
C	-3.658232	0.598572	1.451001
C	-1.872959	1.071783	3.084394
C	0.439611	1.562994	3.637769
C	1.725481	1.027340	2.974515
C	1.498902	1.347219	1.524962
C	0.75663	2.650165	-1.322312

C	-0.126368	2.689344	-2.651726
C	-1.547166	2.257829	-2.387651
C	-3.658232	0.598572	-1.451001
C	-2.901029	0.238592	-2.598889
C	-1.872959	1.071783	-3.084394
C	-0.654562	0.523291	-3.634954
C	0.439611	1.562994	-3.637769
C	1.725481	1.027340	-2.974515
C	1.498902	1.347219	-1.524962
C	1.969866	0.390270	-0.716249
C	1.969866	0.390270	0.716249
C	-0.654562	0.523291	3.634954
C	1.312243	-2.766690	1.171082
C	0.587205	-2.521946	2.305717
C	-0.835811	-2.740120	2.288095
C	-1.481975	-3.270063	1.169259
C	-0.704668	-3.558659	0.000000
C	1.312243	-2.766690	-1.171082
C	2.61355	-2.086356	-0.815819
C	2.61355	-2.086356	0.815819
C	2.690233	-0.689958	1.492429
C	2.113815	-0.507170	2.971259
C	0.934362	-1.486532	3.373708
C	-1.462659	-1.684299	3.029289
C	-2.697886	-1.190003	2.596961
C	-3.366988	-1.739892	1.448541
C	-2.764893	-2.748894	0.739733
C	-2.764893	-2.748894	-0.739733
C	-1.481975	-3.270063	-1.169259

C	-0.835811	-2.740120	-2.288095
C	0.587205	-2.521946	-2.305717
C	2.690233	-0.689958	-1.492429
C	2.113815	-0.507170	-2.971259
C	0.934362	-1.486532	-3.373708
C	-0.433223	-0.819025	-3.556368
C	-1.462659	-1.684299	-3.029289
C	-2.697886	-1.190003	-2.596961
C	-3.366988	-1.739892	-1.448541
C	-4.253212	-0.661280	-0.802981
C	-4.253212	-0.661280	0.802981
C	-0.433223	-0.819025	3.556368
C	-2.901029	0.238592	2.598889
C	0.665193	-3.269917	0.000000
F	3.691691	-2.822909	1.244730
F	3.691691	-2.822909	-1.244730
F	4.029194	-0.345781	-1.533648
F	4.029194	-0.345781	1.533648
F	3.130909	-0.711729	-3.854084
F	3.130909	-0.711729	3.854084
F	1.309444	-2.122680	4.548897
F	1.309444	-2.122680	-4.548897
F	2.795131	1.744098	-3.468043
F	2.795131	1.744098	3.468043
F	0.677032	2.076966	4.884878
F	0.677032	2.076966	-4.884878
F	1.689388	3.677112	-1.433107
F	1.689388	3.677112	1.433107
F	-0.055862	3.932492	3.216318

F	-0.055862	3.932492	-3.216318
F	-5.570866	-0.826558	1.204507
F	-5.570866	-0.826558	-1.204507

6. The relative energies of the non-classical derivatives C_s-C_{58}(NC)F_{18}(A) and C_s-C_{58}(NC)F_{18}(B):

Table S6. The relative energies (kcal/mol) of the non-classical derivatives C_s-C_{58}(NC)F_{18}(A) and C_s-C_{58}(NC)F_{18}(B) at the B3LYP/6-311++G (3*df*, 3*pd*) level.

Molecule	Relative energies
C_s-C_{58}(NC)F_{18}(A)	0.00
C_s-C_{58}(NC)F_{18}(B)	5.567

7. The natural charges of carbon atoms and fluorine atoms of the fluorides C_s-C_{58}(NC)F_{18}(A) and C_s-C_{58}(NC)F_{18}(B):

Table S7. The natural charges of carbon atoms and fluorine atoms of two fluorides C_s-C_{58}(NC)F_{18}(A) and C_s-C_{58}(NC)F_{18}(B) at the B3LYP/6-31G level.

C_s-C_{58}(NC)F_{18}(A)		C_s-C_{58}(NC)F_{18}(B)	
Atom	Natural Charge	Atom	Natural Charge
C (1)	0.33427	C (1)	0.02194
C (2)	-0.01376	C (2)	-0.00592
C (3)	-0.02525	C (3)	0.00184
C (4)	0.34341	C (4)	0.34998
C (5)	0.30916	C (5)	0.31979
C (6)	0.33583	C (6)	-0.02990
C (7)	-0.01376	C (7)	-0.00592
C (8)	0.01443	C (8)	0.00554
C (9)	0.01443	C (9)	0.00554
C (10)	0.00493	C (10)	-0.00197
C (11)	0.01097	C (11)	0.00273
C (12)	0.33562	C (12)	0.33241
C (13)	0.31290	C (13)	0.31157
C (14)	-0.01830	C (14)	-0.00905
C (15)	0.30916	C (15)	0.31979
C (16)	0.34341	C (16)	0.34998
C (17)	-0.02525	C (17)	0.00184

C (18)	0.00493	C (18)	-0.00197
C (19)	0.00463	C (19)	0.01501
C (20)	0.01097	C (20)	0.00273
C (21)	-0.02049	C (21)	-0.02159
C (22)	0.33562	C (22)	0.33241
C (23)	0.31290	C (23)	0.31157
C (24)	-0.01830	C (24)	-0.00905
C (25)	-0.03791	C (25)	-0.03922
C (26)	-0.03791	C (26)	-0.03922
C (27)	-0.02049	C (27)	-0.02159
C (28)	-0.02565	C (28)	-0.02595
C (29)	-0.00689	C (29)	-0.00609
C (30)	0.01767	C (30)	0.01531
C (31)	0.00174	C (31)	-0.00354
C (32)	0.01153	C (32)	0.02599
C (33)	-0.02565	C (33)	-0.02595
C (34)	0.33762	C (34)	0.33769
C (35)	0.33762	C (35)	0.33769
C (36)	0.32324	C (36)	0.32361
C (37)	0.33812	C (37)	0.33822
C (38)	0.33267	C (38)	0.33232
C (39)	0.01459	C (39)	0.00648
C (40)	0.00479	C (40)	0.00307
C (41)	0.00519	C (41)	0.00805
C (42)	0.00649	C (42)	0.00688
C (43)	0.00649	C (43)	0.00688
C (44)	0.00174	C (44)	-0.00354
C (45)	0.01767	C (45)	0.01531
C (46)	-0.00689	C (46)	-0.00609
C (47)	0.32324	C (47)	0.32361
C (48)	0.33812	C (48)	0.33822
C (49)	0.33267	C (49)	0.33232
C (50)	-0.00789	C (50)	-0.00931
C (51)	0.01459	C (51)	0.00648
C (52)	0.00479	C (52)	0.00307
C (53)	0.00519	C (53)	0.00805
C (54)	0.00610	C (54)	0.33915
C (55)	0.00610	C (55)	0.33915
C (56)	-0.00789	C (56)	-0.00931
C (57)	0.00463	C (57)	0.01501
C (58)	0.00309	C (58)	0.00148
F (59)	-0.32592	F (59)	-0.32555
F (60)	-0.32592	F (60)	-0.32555

F (61)	-0.32502	F (61)	-0.32554
F (62)	-0.32502	F (62)	-0.32554
F (63)	-0.31789	F (63)	-0.31798
F (64)	-0.31789	F (64)	-0.31798
F (65)	-0.33432	F (65)	-0.33427
F (66)	-0.33432	F (66)	-0.33427
F (67)	-0.32186	F (67)	-0.32314
F (68)	-0.32186	F (68)	-0.32314
F (69)	-0.32520	F (69)	-0.32612
F (70)	-0.32520	F (70)	-0.32612
F (71)	-0.31533	F (71)	-0.32471
F (72)	-0.31533	F (72)	-0.32471
F (73)	-0.32251	F (73)	-0.32345
F (74)	-0.32251	F (74)	-0.32345
F (75)	-0.31398	F (75)	-0.33600
F (76)	-0.33092	F (76)	-0.33600
Total	0.00000	Total	0.00000

8. The details of calculation:

The non-IPR isomers C_{3v}-$^{\#1205}C_{58}$ and C_2-$^{\#1078}C_{58}$, as well as the non-classical isomer C_s-C_{58}(NC) with its two fluorinated derivatives C_s-C_{58}(NC)F_{18}(A) and C_s-C_{58}(NC)F_{18}(B) have been optimized by Gaussian 09 program at the B3LYP/6-31G** level, with eight-cores CPU (Intel Xeon X5450, 3.0GHz) and 6000MB memory. And then, the single point energies have been calculated by using the 6-311++G (3*df*, 3*pd*) basis set. The total CPU times are listed in Table S8.

Table S8. The total CPU times (hour) for the optimization and single point calculations of the non-IPR isomers C_{3v}-$^{\#1205}C_{58}$ and C_2-$^{\#1078}C_{58}$, as well as the non-classical isomer C_s-C_{58}(NC) with its two fluorides.

Molecule	CPU time (h)
C_{3v}-$^{\#1205}C_{58}$	93.4
C_2-$^{\#1078}C_{58}$	36.6
C_s-C_{58}(NC)	59.7
C_s-C_{58}(NC)F_{18}(A)	115.5
C_s-C_{58}(NC)F_{18}(B)	114.0