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Supporting Information

The Extended Protocol of The Empty $C_2(3)$-C_{82} Fullerene: Isolation, Spectroscopic, Electrochemical and Spectroelectrochemical Characterization and DFT Calculations

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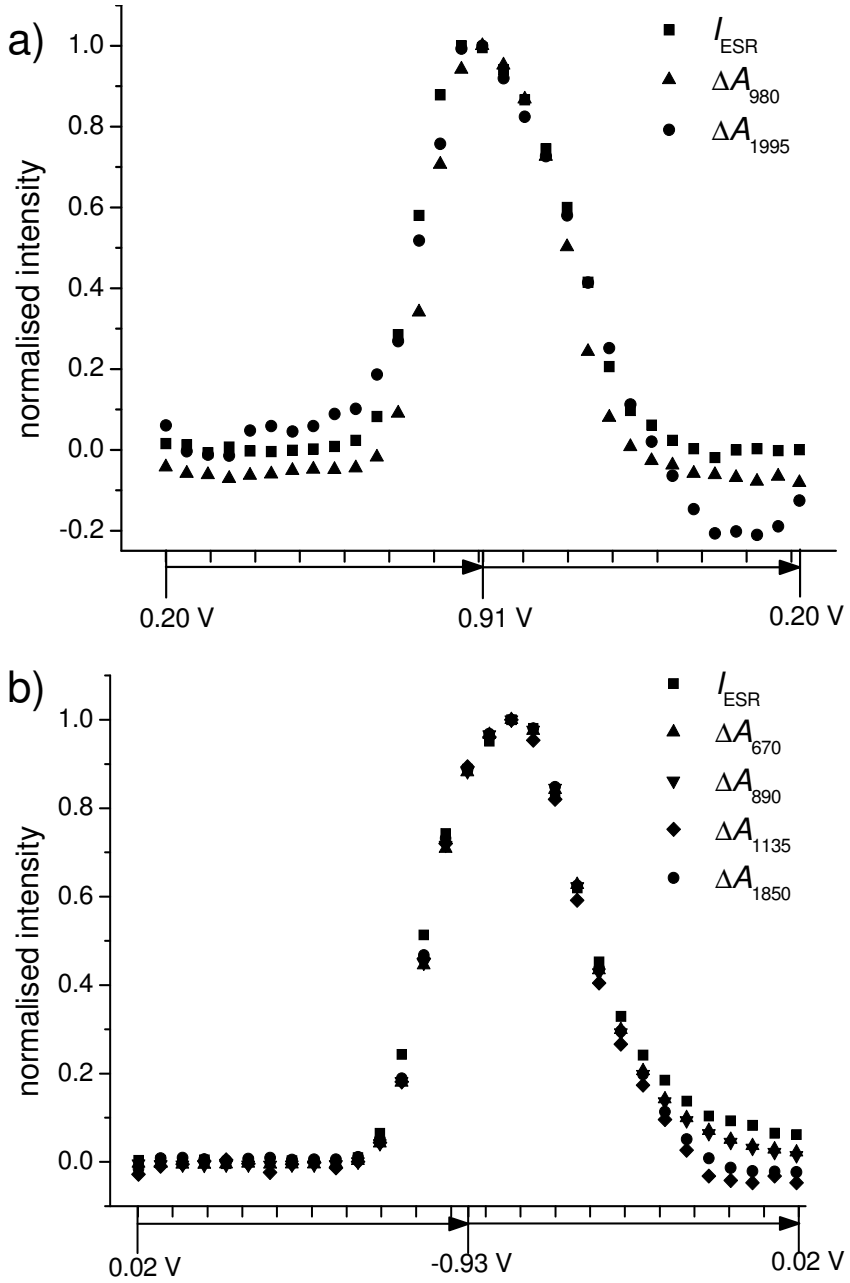
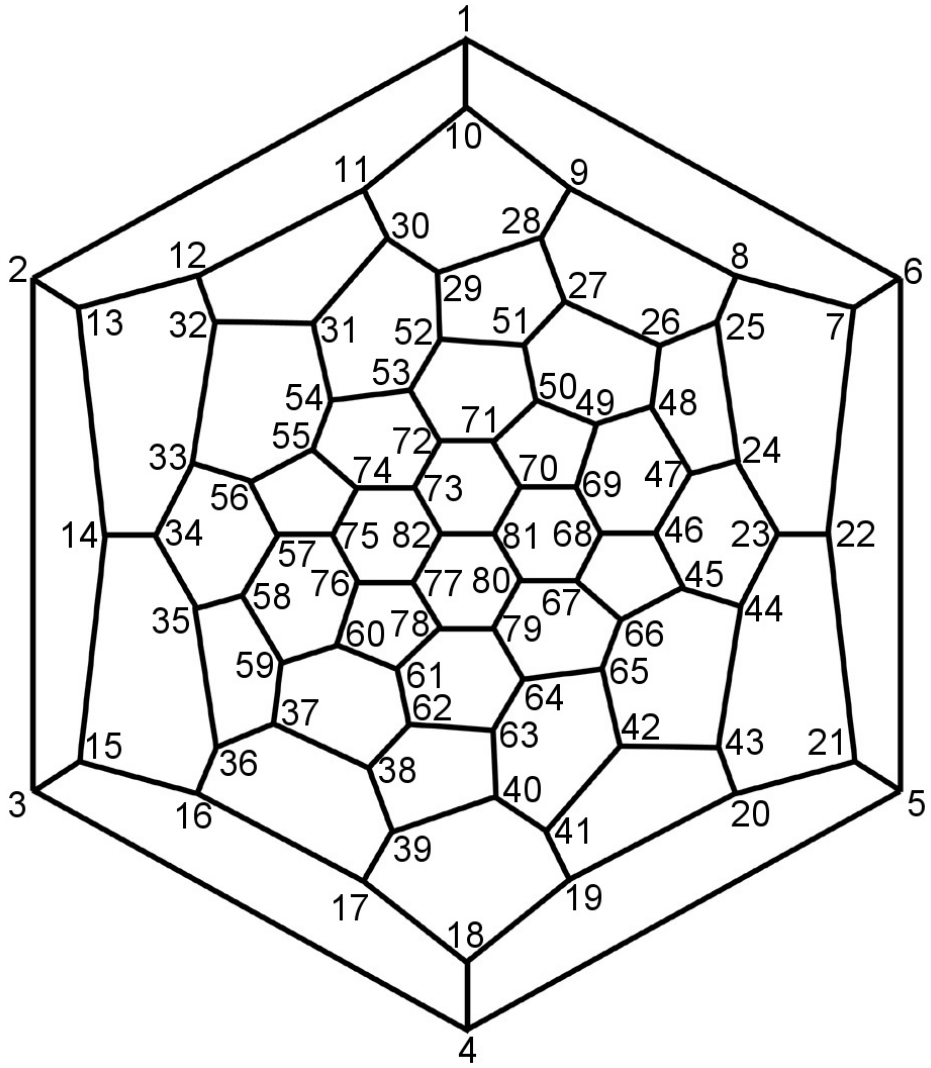


Supporting Information 1 a) relative intensity of the ESR signal (■) and Vis/NIR absorptions at 980 (▲) and 1995 nm (●) of $C_2\,C_{82}$:$3^{+\bullet}$ at different electrode potentials; b) relative intensity of the ESR signal (■) and Vis/NIR absorptions at 670 (▲), 890 (▼), 1135 (♦) and 1850 nm (●) of $C_2\,C_{82}$:$3^{-\bullet}$ at different electrode potentials



Supporting information 2. Schlegel diagram of C_2-C_{82}(3) with IUPAC numbering system used in this work

Supporting information 3. DFT-computed ^{13}C ESR hyperfine constants (in Gauss)

C #	cation	anion	trianion
1	-0.96636	-1.22118	0.01454
2	-0.50754	-0.26266	-0.67937
3	-0.92687	0.19414	-0.51714
4	0.8802	-0.4979	-0.9009
5	-0.50754	-0.39722	-0.55111
6	-0.92687	-1.45838	-1.02495
7	-0.38077	-1.45838	0.16918
8	0.41699	0.18966	1.44276
9	0.68217	-0.23443	0.16918
10	-0.61835	-1.19149	-0.71528
11	0.83032	1.21764	-0.9318
12	-0.46247	0.51266	0.40156
13	-1.82279	-0.14588	-0.11024
14	1.60968	0.1387	-1.02495
15	0.29956	0.51115	-0.00971
16	0.36387	0.27401	-0.56685
17	-0.61237	-0.02449	1.14078
18	-0.61835	-0.14588	-0.40411

C #	cation	anion	trianion
19	0.68217	-0.17004	-0.51714
20	1.60968	0.54247	0.7689
21	-0.96636	-0.04742	-0.9318
22	0.41536	-0.24738	0.02232
23	-0.46247	-0.23443	-0.40411
24	-1.82279	0.33967	-0.94584
25	-0.30376	-0.39368	-0.18239
26	-0.01423	0.39753	-0.45547
27	0.8802	-0.10883	0.02232
28	-0.61237	-0.17004	1.44276
29	0.41536	-1.19149	1.14078
30	-1.53611	-0.80295	-0.55111
31	-1.84259	1.24266	-0.11024
32	2.77772	0.59275	0.6791
33	-2.08891	-0.09228	-0.61438
34	-0.01423	-0.9158	-0.00971
35	0.41825	-0.09228	-0.56685
36	-0.38077	-0.08088	1.26856
37	0.41699	0.24094	0.53403
38	-0.30376	-0.26266	0.04537
39	0.36387	0.54247	0.40645
40	-1.53611	0.51115	0.41527
41	0.83032	-0.08088	1.35279
42	-1.84259	0.42448	0.7689
43	2.77772	0.1387	-0.91044
44	-2.08891	0.42448	-0.73509
45	2.14757	0.27401	-0.61438
46	-1.18002	-0.42668	-0.71528
47	0.20054	-0.4979	0.14252
48	0.50629	-0.13092	0.04537
49	-0.61856	-0.39368	1.09137
50	0.29956	1.21764	-1.3954
51	-0.09387	-0.24738	-1.01056
52	-1.13884	0.51266	-0.73509
53	-1.71594	-0.42668	0.40645
54	0.4589	1.24266	-0.91044
55	-1.55321	0.59275	-0.45547
56	2.14757	1.51361	-0.47102
57	-0.61856	-0.10883	-1.01056
58	0.20054	-0.80295	-0.18239
59	-1.18002	-0.13092	0.01454
60	-1.13884	-0.89837	1.09137
61	-0.09387	-0.64709	-0.49906
62	-0.27242	-0.57154	-0.67937
63	-1.71594	0.24094	-0.47102
64	0.41825	-0.39722	1.232
65	0.4589	-1.03454	0.14252
66	-1.55321	-0.64709	1.232
67	2.0421	-0.02449	-1.3954
68	-0.53979	-1.22118	0.26046
69	-0.04157	0.18966	-0.35152
70	0.69088	1.51361	0.53403
71	2.46262	0.33967	1.26856

C #		cation	anion	trianion
	72	-0.27242	0.39753	0.6791
	73	-1.52117	-0.41605	0.40156
	74	2.0421	-0.41605	-0.49906
	75	-0.53979	-0.9158	0.41527
	76	-0.04157	-0.89837	-0.94584
	77	0.69088	0.26932	1.35279
	78	0.50629	-0.04742	0.26046
	79	2.46262	0.19414	-0.35152
	80	-1.52117	-0.57154	-0.70809
	81	-0.46582	0.26932	-0.70809
	82	-0.46582	-1.03454	-0.9009