

--- Supporting Information for: ---

Th@C₈₆, Th@C₈₂, Th@C₈₀, and Th@C₇₆. Role of Thorium Encapsulation in Determining Spherical Aromatic and Bonding Properties on Medium-Sized Endohedral Metallic Fullerenes

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Content:

Table S1. Coordinates and shielding tensor parameters for all carbon atoms for Th@C₇₆, Th@C₈₀, Th@C₈₂, and Th@C₈₆. Summarized values are given on main text.

Figure S1. Most shielded carbon atoms of Th@C₈₂.

Table S2. Energy decomposition analysis for the Th-Fullerene interaction. Values in kcal mol⁻¹.

Th@C₇₆

	X	Y	Z	σ_{11}	σ_{22}	σ_{33}	σ_{iso}	σ_{anis}	σ_{asym}	δ vs TMS	δ vs C ₆₀
C	-3.2178	0.7264	2.8193	-25.8	-10.6	138.7	34.1	156.9	0.15	152.6	147.2
C	-3.2178	-0.7264	2.8193	-25.8	-10.6	138.7	34.1	156.9	0.15	152.6	147.2
C	0.9798	-3.1499	2.8193	-25.8	-10.5	138.7	34.1	156.8	0.15	152.6	147.2
C	0.9798	3.1499	2.8193	-25.8	-10.5	138.7	34.1	156.8	0.15	152.6	147.2
C	2.2380	2.4235	2.8193	-25.7	-10.5	138.7	34.2	156.7	0.15	152.5	147.1
C	2.2380	-2.4235	2.8193	-25.7	-10.5	138.7	34.2	156.7	0.15	152.5	147.1
C	-1.4064	0.0000	4.0592	-38.0	14.4	130.2	35.5	142.0	0.55	151.1	145.7
C	0.7032	1.2180	4.0592	-37.9	14.5	130.2	35.6	141.9	0.55	151.1	145.7
C	0.7032	-1.2180	4.0592	-37.9	14.5	130.2	35.6	141.9	0.55	151.1	145.7
C	3.0539	-2.4423	1.6876	-25.3	-11.8	145.7	36.2	164.2	0.12	150.5	145.1
C	3.0539	2.4423	1.6876	-25.3	-11.8	145.7	36.2	164.2	0.12	150.5	145.1
C	0.5882	3.8659	1.6876	-25.3	-11.8	145.7	36.2	164.2	0.12	150.5	145.1
C	0.5882	-3.8659	1.6876	-25.3	-11.8	145.7	36.2	164.2	0.12	150.5	145.1
C	-3.6421	1.4236	1.6876	-25.3	-11.7	145.6	36.2	164.1	0.12	150.5	145.1
C	-3.6421	-1.4236	1.6876	-25.3	-11.7	145.6	36.2	164.1	0.12	150.5	145.1
C	0.9444	3.0993	-1.7945	-13.1	-8.1	139.8	39.5	150.4	0.05	147.2	141.8
C	0.9444	-3.0993	-1.7945	-13.1	-8.1	139.8	39.5	150.4	0.05	147.2	141.8
C	-3.1563	0.7317	-1.7945	-13.1	-8.1	139.8	39.5	150.4	0.05	147.1	141.8
C	-3.1563	-0.7317	-1.7945	-13.1	-8.1	139.8	39.5	150.4	0.05	147.1	141.8

C	2.2118	2.3675	-1.7945	-13.1	-8.1	139.8	39.5	150.4	0.05	147.1	141.8
C	2.2118	-2.3675	-1.7945	-13.1	-8.1	139.8	39.5	150.4	0.05	147.1	141.8
C	-1.7808	-3.0844	2.0027	-22.2	-1.9	143.1	39.7	155.1	0.20	147.0	141.6
C	-1.7808	3.0844	2.0027	-22.2	-1.9	143.1	39.7	155.1	0.20	147.0	141.6
C	3.5616	0.0000	2.0027	-22.1	-1.8	143.1	39.7	155.1	0.20	147.0	141.6
C	2.7072	0.0000	3.2027	-16.9	-4.1	141.0	40.0	151.5	0.13	146.7	141.3
C	-1.3536	-2.3445	3.2027	-17.0	-4.0	141.0	40.0	151.5	0.13	146.7	141.3
C	-1.3536	2.3445	3.2027	-17.0	-4.0	141.0	40.0	151.5	0.13	146.7	141.3
C	2.6448	-3.1720	0.5173	-23.8	-3.7	150.0	40.8	163.8	0.18	145.8	140.4
C	2.6448	3.1720	0.5173	-23.8	-3.7	150.0	40.8	163.8	0.18	145.8	140.4
C	1.4247	-3.8765	0.5173	-23.8	-3.7	150.0	40.8	163.8	0.18	145.8	140.4
C	1.4247	3.8765	0.5173	-23.8	-3.7	150.0	40.9	163.8	0.18	145.8	140.4
C	-4.0695	0.7044	0.5173	-23.8	-3.7	150.0	40.9	163.7	0.18	145.8	140.4
C	-4.0695	-0.7044	0.5173	-23.8	-3.7	150.0	40.9	163.7	0.18	145.8	140.4
C	-2.0865	-1.1782	3.5765	-19.0	2.4	145.3	42.9	153.6	0.21	143.8	138.4
C	-2.0865	1.1782	3.5765	-19.0	2.4	145.3	42.9	153.6	0.21	143.8	138.4
C	2.0636	-1.2179	3.5765	-19.0	2.5	145.3	42.9	153.5	0.21	143.8	138.4
C	2.0636	1.2179	3.5765	-19.0	2.5	145.3	42.9	153.5	0.21	143.8	138.4
C	0.0229	-2.3961	3.5765	-19.0	2.5	145.3	42.9	153.6	0.21	143.7	138.3
C	0.0229	2.3961	3.5765	-19.0	2.5	145.3	42.9	153.6	0.21	143.7	138.3
C	-2.9073	-2.5997	1.2674	-20.7	6.1	145.2	43.6	152.5	0.26	143.1	137.7
C	-2.9073	2.5997	1.2674	-20.7	6.1	145.2	43.6	152.5	0.26	143.1	137.7
C	-0.7978	3.8177	1.2674	-20.6	6.3	145.2	43.6	152.4	0.26	143.0	137.6
C	-0.7978	-3.8177	1.2674	-20.6	6.3	145.2	43.6	152.4	0.26	143.0	137.6
C	3.7051	-1.2179	1.2674	-20.6	6.3	145.3	43.6	152.4	0.26	143.0	137.6
C	3.7051	1.2179	1.2674	-20.6	6.3	145.3	43.7	152.4	0.26	143.0	137.6
C	-1.4775	2.5591	-2.1169	-2.6	0.9	132.9	43.7	133.8	0.04	143.0	137.6
C	-1.4775	-2.5591	-2.1169	-2.6	0.9	132.9	43.7	133.8	0.04	143.0	137.6
C	2.9549	0.0000	-2.1169	-2.5	0.8	132.9	43.7	133.8	0.04	143.0	137.6
C	-3.5974	-1.4173	-0.6369	-22.4	18.0	145.6	47.1	147.8	0.41	139.6	134.2
C	-3.5974	1.4173	-0.6369	-22.4	18.0	145.6	47.1	147.8	0.41	139.6	134.2
C	3.0261	2.4068	-0.6369	-22.5	18.1	145.6	47.1	147.7	0.41	139.6	134.2
C	3.0261	-2.4068	-0.6369	-22.5	18.1	145.6	47.1	147.7	0.41	139.6	134.2
C	0.5713	3.8241	-0.6369	-22.5	18.1	145.6	47.1	147.7	0.41	139.6	134.2
C	0.5713	-3.8241	-0.6369	-22.5	18.1	145.6	47.1	147.7	0.41	139.6	134.2
C	0.0008	1.4551	-3.5397	3.1	22.2	130.2	51.8	117.6	0.24	134.9	129.5
C	0.0008	-1.4551	-3.5397	3.1	22.2	130.2	51.8	117.6	0.24	134.9	129.5
C	-1.2606	0.7268	-3.5397	3.1	22.3	130.2	51.9	117.5	0.25	134.8	129.4
C	-1.2606	-0.7268	-3.5397	3.1	22.3	130.2	51.9	117.5	0.25	134.8	129.4
C	1.2597	0.7283	-3.5397	3.1	22.2	130.2	51.9	117.5	0.24	134.8	129.4
C	1.2597	-0.7283	-3.5397	3.1	22.2	130.2	51.9	117.5	0.24	134.8	129.4
C	3.7348	-1.2180	-0.1627	-18.8	40.5	135.1	52.3	124.3	0.72	134.4	129.0
C	3.7348	1.2180	-0.1627	-18.8	40.5	135.1	52.3	124.3	0.72	134.4	129.0

C	-2.9222	-2.6255	-0.1627	-18.8	40.5	135.1	52.3	124.3	0.72	134.4	129.0
C	-2.9222	2.6255	-0.1627	-18.8	40.5	135.1	52.3	124.3	0.72	134.4	129.0
C	-0.8126	3.8435	-0.1627	-18.8	40.6	135.1	52.3	124.2	0.72	134.4	129.0
C	-0.8126	-3.8435	-0.1627	-18.8	40.6	135.1	52.3	124.2	0.72	134.4	129.0
C	0.0000	0.0000	4.2624	-0.3	-0.3	159.5	53.0	159.8	0.00	133.7	128.3
C	2.2803	1.1649	-2.6117	8.7	18.2	133.2	53.4	119.8	0.12	133.3	127.9
C	2.2803	-1.1649	-2.6117	8.7	18.2	133.2	53.4	119.8	0.12	133.3	127.9
C	-0.1313	2.5572	-2.6117	8.7	18.2	133.2	53.4	119.7	0.12	133.3	127.9
C	-0.1313	-2.5572	-2.6117	8.7	18.2	133.2	53.4	119.7	0.12	133.3	127.9
C	-2.1490	1.3923	-2.6117	8.7	18.3	133.2	53.4	119.7	0.12	133.3	127.9
C	-2.1490	-1.3923	-2.6117	8.7	18.2	133.2	53.4	119.7	0.12	133.3	127.9
C	-1.8374	3.1824	-0.8798	-4.4	3.1	165.4	54.7	166.0	0.07	132.0	126.6
C	-1.8374	-3.1824	-0.8798	-4.4	3.1	165.4	54.7	166.0	0.07	132.0	126.6
C	3.6747	0.0000	-0.8798	-4.4	3.1	165.4	54.7	166.0	0.07	132.0	126.6
Th	0.0000	0.0000	-1.5022								

Th@C₈₀

	X	Y	Z	σ_{11}	σ_{22}	σ_{33}	σ_{iso}	σ_{anis}	σ_{asym}	δ vs TMS	δ vs C ₆₀
C	-3.2410	-0.5586	-2.4141	-44.3	-38.8	135.7	17.5	177.2	0.05	169.2	163.8
C	-3.6723	-1.5940	-0.2575	-43.9	-18.1	137.0	25.0	168.0	0.23	161.7	156.3
C	1.9585	-3.5174	-0.4144	-38.2	-29.5	144.8	25.7	178.6	0.07	160.9	155.6
C	0.1899	-3.9444	1.2220	-49.1	-16.9	145.2	26.4	178.2	0.27	160.3	154.9
C	-0.2166	0.6174	4.6506	-33.6	-11.9	126.7	27.1	149.4	0.22	159.6	154.2
C	-0.9273	1.5809	-4.0984	-45.6	-17.2	144.9	27.4	176.2	0.24	159.3	153.9
C	-0.4714	2.8564	-3.5816	-43.7	-21.4	147.8	27.6	180.3	0.19	159.1	153.7
C	-1.7132	-3.5518	-0.8535	-37.2	-26.4	146.7	27.7	178.5	0.09	159.0	153.6
C	-1.2943	1.3553	4.0517	-34.3	-18.0	137.6	28.4	163.7	0.15	158.2	152.9
C	-2.4270	2.8969	-2.0652	-34.1	-31.0	150.6	28.5	183.1	0.03	158.2	152.8
C	-1.1999	3.4889	-2.5557	-39.9	-21.2	148.3	29.1	178.9	0.16	157.6	152.2
C	-0.5166	-0.8067	4.5354	-32.8	-20.1	141.1	29.4	167.5	0.11	157.3	151.9
C	-2.2762	-0.3645	-3.4669	-35.8	-23.5	151.4	30.7	181.1	0.10	156.0	150.6
C	0.9705	2.8089	-3.5132	-41.1	-16.4	150.1	30.9	178.9	0.21	155.8	150.4
C	2.5397	-0.5280	-3.2456	-36.5	-23.1	153.8	31.4	183.6	0.11	155.3	149.9
C	-0.3310	-3.8092	-1.1685	-27.0	-19.5	141.7	31.7	164.9	0.07	154.9	149.6
C	1.6459	3.3886	-2.4298	-32.3	-21.6	149.8	32.0	176.8	0.09	154.7	149.3
C	-3.8937	-0.2905	0.3080	-40.6	-16.3	153.0	32.1	181.5	0.20	154.6	149.2
C	-0.0155	-3.1111	-2.3904	-31.6	-24.9	152.7	32.1	181.0	0.05	154.6	149.2
C	3.4422	-0.7705	-2.1398	-42.8	-3.5	143.2	32.3	166.4	0.35	154.4	149.0
C	2.2768	-2.8650	-1.6587	-29.9	-17.9	149.9	34.0	173.7	0.10	152.6	147.3
C	-2.2495	-2.7168	-1.8958	-24.5	-15.3	142.4	34.2	162.3	0.09	152.5	147.1
C	3.5489	-1.8689	0.0363	-30.2	-18.4	151.3	34.2	175.6	0.10	152.5	147.1
C	0.2212	0.7068	-4.2694	-31.1	-16.8	152.9	35.0	176.8	0.12	151.7	146.3

C	-1.2037	-2.4508	-2.8500	-31.3	-14.5	152.6	35.6	175.5	0.14	151.1	145.7
C	-3.5708	0.7391	-1.8552	-40.7	0.1	147.9	35.8	168.2	0.36	150.9	145.5
C	3.3147	-1.9170	-1.3790	-39.9	-4.7	153.4	36.3	175.7	0.30	150.4	145.0
C	-3.1711	-2.4528	0.7797	-24.4	-18.0	152.5	36.7	173.6	0.06	150.0	144.6
C	-1.8453	-0.8908	3.9125	-25.0	4.4	130.8	36.7	141.2	0.31	149.9	144.5
C	2.7622	-2.9234	0.6353	-35.1	-0.1	146.2	37.0	163.8	0.32	149.7	144.3
C	-2.4726	3.0351	-0.6263	-25.4	-9.4	146.9	37.4	164.3	0.15	149.3	143.9
C	-1.1904	-3.6757	1.5389	-21.8	-14.8	149.5	37.6	167.8	0.06	149.0	143.7
C	1.3920	1.5012	-3.9928	-43.6	7.0	149.9	37.8	168.2	0.45	148.9	143.5
C	-3.5695	-0.3451	1.6893	-40.9	2.4	152.3	37.9	171.6	0.38	148.7	143.4
C	0.5355	-1.7133	4.1053	-16.9	-5.5	136.7	38.1	147.9	0.12	148.6	143.2
C	3.2480	1.5224	-2.3727	-31.4	-4.4	150.2	38.1	168.1	0.24	148.5	143.1
C	-2.1367	1.0487	-3.6714	-43.9	9.4	150.3	38.6	167.5	0.48	148.1	142.7
C	2.7845	2.7158	-1.8358	-32.7	-4.3	153.5	38.8	171.9	0.25	147.9	142.5
C	-0.7784	2.3890	3.2113	-22.6	-6.5	146.2	39.0	160.7	0.15	147.7	142.3
C	3.2868	-0.5469	2.0353	-20.4	-7.7	145.7	39.2	159.7	0.12	147.5	142.1
C	0.8894	3.9734	-1.3472	-31.2	-1.0	150.7	39.5	166.8	0.27	147.2	141.8
C	1.0126	1.2187	4.1878	-16.7	-8.5	143.8	39.5	156.3	0.08	147.2	141.8
C	2.5215	0.8922	-3.4643	-37.3	6.1	151.9	40.2	167.5	0.39	146.4	141.0
C	-2.9170	1.7311	-2.6527	-32.8	3.0	150.7	40.3	165.6	0.32	146.4	141.0
C	3.7648	0.4890	-1.5146	-32.7	1.3	152.9	40.5	168.6	0.30	146.1	140.8
C	-2.1477	-3.4160	0.4983	-20.1	-7.5	149.3	40.6	163.2	0.12	146.1	140.7
C	-2.2937	0.4582	3.5828	-16.3	-12.1	150.8	40.8	165.0	0.04	145.9	140.5
C	1.0025	-3.3973	2.2645	-24.8	-3.7	151.2	40.9	165.4	0.19	145.8	140.4
C	2.7152	2.8576	-0.3989	-29.3	6.5	147.4	41.5	158.9	0.34	145.2	139.8
C	0.6742	2.3195	3.2959	-11.6	10.9	127.3	42.2	127.6	0.26	144.5	139.1
C	-3.7141	0.9030	-0.4490	-21.2	-8.0	157.6	42.8	172.2	0.11	143.9	138.5
C	3.7512	0.6162	-0.0976	-19.9	-5.8	154.1	42.8	166.9	0.13	143.9	138.5
C	1.2720	-2.5612	-2.6322	-25.3	-1.6	157.6	43.6	171.1	0.21	143.1	137.7
C	-1.1507	-1.2420	-3.5944	-24.4	-2.2	158.3	43.9	171.6	0.19	142.8	137.4
C	1.3789	-1.3355	-3.4331	-16.4	-8.3	157.8	44.4	170.1	0.07	142.3	136.9
C	-0.4992	4.0221	-1.4130	-34.1	15.7	151.6	44.4	160.7	0.46	142.3	136.9
C	-3.2274	-1.7238	-1.6064	-16.8	-10.7	163.3	45.3	177.0	0.05	141.4	136.0
C	2.2705	-2.8124	1.9561	-18.5	-2.3	159.0	46.1	169.4	0.14	140.6	135.2
C	2.6289	-1.6390	2.7013	-12.5	7.1	144.2	46.3	146.9	0.20	140.4	135.0
C	1.5409	3.6387	-0.0971	-31.1	20.3	150.5	46.6	155.9	0.49	140.1	134.7
C	-1.2746	3.7275	-0.2241	-36.9	26.9	150.5	46.8	155.5	0.62	139.8	134.4
C	2.0521	0.3341	3.7939	-10.6	20.0	133.3	47.6	128.6	0.36	139.1	133.7
C	0.1615	-0.6813	-3.9417	-13.2	-1.4	157.8	47.8	165.1	0.11	138.9	133.5
C	-1.2293	-2.9805	2.7880	-14.0	10.4	147.4	47.9	149.2	0.25	138.7	133.4
C	2.6168	1.8370	1.8183	-4.7	1.4	151.2	49.3	152.8	0.06	137.4	132.0
C	0.6410	-3.9748	-0.1405	-12.8	-1.3	163.0	49.6	170.0	0.10	137.0	131.7
C	-2.2089	-1.9699	3.0310	-16.4	5.1	160.9	49.9	166.6	0.19	136.8	131.4

C	-2.6180	1.9512	1.5790	-7.9	7.5	150.2	49.9	150.3	0.15	136.7	131.4
C	-3.1585	-1.7076	2.0073	-9.9	14.0	148.5	50.9	146.4	0.24	135.8	130.4
C	1.8385	-1.1174	3.7967	-8.9	30.5	134.0	51.9	123.2	0.48	134.8	129.4
C	3.7192	-0.6162	0.6806	-5.7	-0.7	164.0	52.6	167.2	0.04	134.1	128.7
C	-3.0789	2.0510	0.2019	-5.4	4.7	159.0	52.8	159.3	0.10	133.9	128.5
C	-0.6646	3.4597	1.0117	-4.5	10.1	155.5	53.7	152.7	0.14	133.0	127.6
C	3.1763	1.8393	0.4780	-4.6	5.3	161.7	54.1	161.4	0.09	132.5	127.2
C	1.4609	2.6550	2.1317	-11.8	17.5	156.9	54.2	154.0	0.29	132.5	127.1
C	0.1395	-2.8044	3.2617	-7.8	24.2	147.5	54.6	139.2	0.34	132.0	126.6
C	2.8461	0.6720	2.6404	-0.9	19.5	147.5	55.4	138.2	0.22	131.3	125.9
C	0.8074	3.4202	1.0876	2.1	14.5	156.5	57.7	148.2	0.12	129.0	123.6
C	-1.4433	2.7153	1.9842	5.4	11.0	156.9	57.8	148.7	0.06	128.9	123.5
C	-2.9891	0.7589	2.3621	0.6	33.2	154.4	62.7	137.5	0.36	124.0	118.6
Th	0.0000	0.0000	2.1561								

Th@C₈₂

	X	Y	Z	σ_{11}	σ_{22}	σ_{33}	σ_{iso}	σ_{anis}	σ_{asym}	δ vs TMS	δ vs C ₆₀	
C	-1.3141	3.3578	2.6360	-45.4	5.1	142.1	33.9	162.3	0.47	152.8	147.4	Average
C	-1.3141	3.3578	-2.6360	-45.4	5.1	142.1	33.9	162.3	0.47	152.8	147.4	147.4
C	-2.6567	0.1067	3.1621	-32.3	-10.3	144.4	33.9	165.7	0.20	152.7	147.4	Exp.
C	-2.6567	0.1067	-3.1621	-32.3	-10.3	144.4	33.9	165.7	0.20	152.7	147.4	148.5
C	3.2429	3.0779	0.0000	-45.4	5.5	142.1	34.0	162.0	0.47	152.7	147.3	
C	-1.4034	0.0297	-3.8878	-32.2	-9.8	144.3	34.1	165.3	0.20	152.6	147.2	
C	-1.4034	0.0297	3.8878	-32.2	-9.8	144.3	34.1	165.3	0.20	152.6	147.2	
C	4.0628	-0.3062	0.7253	-32.1	-9.5	144.5	34.3	165.3	0.20	152.4	147.0	
C	4.0628	-0.3062	-0.7253	-32.1	-9.5	144.5	34.3	165.3	0.20	152.4	147.0	
C	-2.8488	1.4673	2.7406	-27.6	-15.8	150.4	35.7	172.1	0.10	151.0	145.6	Average
C	-2.8488	1.4673	-2.7406	-27.6	-15.8	150.4	35.7	172.1	0.10	151.0	145.6	145.6
C	-0.8188	1.3430	3.9153	-27.6	-15.8	150.5	35.7	172.2	0.10	151.0	145.6	Exp.
C	-0.8188	1.3430	-3.9153	-27.6	-15.8	150.5	35.7	172.2	0.10	151.0	145.6	146.3
C	3.9183	1.0517	1.1742	-27.4	-15.5	150.4	35.8	171.8	0.10	150.9	145.5	
C	3.9183	1.0517	-1.1742	-27.4	-15.5	150.4	35.8	171.8	0.10	150.9	145.5	
C	0.2998	4.4714	1.4196	-40.5	-1.0	150.7	36.4	171.5	0.35	150.3	144.9	Average
C	0.2998	4.4714	-1.4196	-40.5	-1.0	150.7	36.4	171.5	0.35	150.3	144.9	144.8
C	1.4964	4.3981	-0.7278	-40.3	-1.0	150.7	36.5	171.4	0.34	150.2	144.8	Exp.
C	1.4964	4.3981	0.7278	-40.3	-1.0	150.7	36.5	171.4	0.34	150.2	144.8	146.1
C	-0.9584	4.5485	0.6920	-40.5	-0.7	150.7	36.5	171.3	0.35	150.2	144.8	
C	-0.9584	4.5485	-0.6920	-40.4	-0.7	150.7	36.5	171.3	0.35	150.2	144.8	
C	-1.7572	2.2262	3.2823	-42.6	0.0	155.7	37.7	177.0	0.36	149.0	143.6	Average
C	-1.7572	2.2262	-3.2823	-42.6	0.0	155.7	37.7	177.0	0.36	149.0	143.6	143.6
C	3.9164	1.8775	0.0000	-42.5	-0.1	155.7	37.7	177.0	0.36	149.0	143.6	Exp.
C	-3.9393	0.7060	0.7188	-21.1	-13.8	148.5	37.9	166.0	0.07	148.8	143.4	145.1

C	-3.9393	0.7060	-0.7188	-21.1	-13.8	148.5	37.9	166.0	0.07	148.8	143.4	
C	2.6405	0.3024	3.0878	-21.0	-13.7	148.4	37.9	165.7	0.07	148.8	143.4	
C	2.6405	0.3024	-3.0878	-21.0	-13.7	148.4	37.9	165.7	0.07	148.8	143.4	
C	1.3979	0.3786	3.8064	-21.0	-13.7	148.5	37.9	165.9	0.07	148.7	143.3	
C	1.3979	0.3786	-3.8064	-21.0	-13.7	148.5	38.0	165.9	0.07	148.7	143.3	
C	-2.3059	-2.1619	-2.3405	-20.0	-12.4	146.4	38.0	162.6	0.07	148.7	143.3	Average
C	-2.3059	-2.1619	2.3405	-20.0	-12.4	146.4	38.0	162.6	0.07	148.7	143.3	143.3
C	-1.0742	-2.2379	3.0532	-19.6	-12.1	146.3	38.2	162.1	0.07	148.5	143.1	Exp.
C	-1.0742	-2.2379	-3.0532	-19.6	-12.1	146.3	38.2	162.1	0.07	148.5	143.1	144.9
C	2.9679	-2.4850	0.7123	-19.0	-12.0	146.2	38.4	161.7	0.06	148.3	142.9	
C	2.9679	-2.4850	-0.7123	-19.0	-12.0	146.2	38.4	161.7	0.06	148.3	142.9	
C	0.0993	3.6594	2.5854	-22.6	-13.5	153.7	39.2	171.7	0.08	147.5	142.1	Average
C	0.0993	3.6594	-2.5854	-22.6	-13.5	153.7	39.2	171.7	0.08	147.5	142.1	142.1
C	-1.9414	3.7847	-1.4053	-22.5	-13.5	153.7	39.2	171.7	0.08	147.4	142.0	Exp.
C	-1.9414	3.7847	1.4053	-22.5	-13.5	153.7	39.2	171.7	0.08	147.4	142.0	142.4
C	2.5287	3.5105	1.1803	-22.2	-13.4	153.8	39.4	171.6	0.08	147.3	141.9	
C	2.5287	3.5105	-1.1803	-22.2	-13.4	153.8	39.4	171.6	0.08	147.3	141.9	
C	-3.8047	-0.6504	-1.1630	-19.8	-7.3	146.8	39.9	160.4	0.12	146.8	141.4	Average
C	-3.8047	-0.6504	1.1630	-19.8	-7.3	146.8	39.9	160.4	0.12	146.8	141.4	141.4
C	2.8335	-1.0577	2.6773	-20.0	-6.8	146.8	40.0	160.2	0.12	146.7	141.3	Exp.
C	2.8335	-1.0577	-2.6773	-20.0	-6.8	146.8	40.0	160.2	0.12	146.7	141.3	141.4
C	-0.2497	-4.1344	0.0000	-10.6	-10.3	141.2	40.1	151.6	0.00	146.6	141.2	
C	0.8225	-0.9342	3.8400	-19.5	-6.9	146.8	40.1	160.1	0.12	146.5	141.2	
C	0.8225	-0.9342	-3.8400	-19.5	-6.9	146.8	40.1	160.1	0.12	146.5	141.2	
C	1.7001	-1.8334	3.1266	-17.5	0.0	147.7	43.4	156.5	0.17	143.3	137.9	Average
C	1.7001	-1.8334	-3.1266	-17.5	0.0	147.7	43.4	156.5	0.17	143.3	137.9	137.8
C	-3.7061	-1.5018	0.0000	-17.3	-0.6	148.2	43.4	157.2	0.16	143.2	137.8	Exp. 136.9
C	-2.8883	2.9566	0.7334	-16.5	-5.6	157.5	45.1	168.5	0.10	141.6	136.2	Average
C	-2.8883	2.9566	-0.7334	-16.5	-5.6	157.5	45.1	168.5	0.10	141.6	136.2	136.1
C	1.1899	-3.8687	0.0000	-4.3	6.6	133.2	45.2	132.0	0.12	141.5	136.1	Exp.
C	1.0721	2.7133	-3.0238	-16.5	-5.5	157.5	45.2	168.5	0.10	141.5	136.1	136.5
C	1.0721	2.7133	3.0238	-16.5	-5.5	157.5	45.2	168.5	0.10	141.5	136.1	
C	2.3398	2.6355	2.2904	-16.3	-5.5	157.5	45.2	168.4	0.10	141.5	136.1	
C	2.3398	2.6355	-2.2904	-16.3	-5.5	157.5	45.2	168.4	0.10	141.5	136.1	
C	-3.3915	1.7884	1.4600	-20.9	-2.3	158.8	45.2	170.4	0.16	141.4	136.1	
C	-3.3915	1.7884	-1.4600	-20.9	-2.3	158.8	45.2	170.4	0.16	141.4	136.1	
C	0.5857	1.5445	3.7605	-20.7	-2.2	158.8	45.3	170.3	0.16	141.4	136.0	
C	0.5857	1.5445	-3.7605	-20.7	-2.2	158.8	45.3	170.3	0.16	141.4	136.0	
C	3.1093	1.3896	2.3006	-20.4	-2.1	158.9	45.5	170.2	0.16	141.2	135.8	
C	3.1093	1.3896	-2.3006	-20.4	-2.1	158.9	45.5	170.2	0.16	141.2	135.8	
C	-0.9349	-3.7315	1.2284	-4.1	8.0	133.6	45.8	131.6	0.14	140.8	135.5	
C	-0.9349	-3.7315	-1.2284	-4.1	8.0	133.6	45.8	131.6	0.14	140.8	135.5	
C	-2.9019	-2.6712	0.0000	-9.4	12.0	147.9	50.2	146.6	0.22	136.5	131.1	Average
C	1.1968	-2.9263	2.3728	-8.5	12.2	147.2	50.3	145.4	0.21	136.4	131.0	131.0
C	1.1968	-2.9263	-2.3728	-8.5	12.2	147.2	50.3	145.4	0.21	136.4	131.0	Exp. 130.9

C	1.8750	-3.2957	-1.1629	-0.3	16.0	139.1	51.6	131.2	0.19	135.1	129.7	Average
C	1.8750	-3.2957	1.1629	-0.3	16.0	139.1	51.6	131.2	0.19	135.1	129.7	129.4
C	-2.2255	-3.0387	1.2101	-0.2	16.2	139.6	51.9	131.6	0.19	134.8	129.4	Exp. 130.9
C	-2.2255	-3.0387	-1.2101	-0.2	16.2	139.6	51.9	131.6	0.19	134.8	129.4	
C	-0.2177	-3.1655	2.3745	-0.4	17.0	139.4	52.0	131.0	0.20	134.7	129.3	
C	-0.2177	-3.1655	-2.3745	-0.4	17.0	139.4	52.0	131.0	0.20	134.7	129.3	
C	-0.5837	-1.1199	3.8089	-4.7	12.2	162.6	56.7	158.8	0.16	130.0	124.6	Average
C	-0.5837	-1.1199	-3.8089	-4.7	12.2	162.6	56.7	158.8	0.16	130.0	124.6	124.4
C	-3.0991	-0.9656	2.3528	-4.5	12.5	162.7	56.9	158.7	0.16	129.8	124.4	Exp. 128.5
C	-3.0991	-0.9656	-2.3528	-4.5	12.5	162.7	56.9	158.7	0.16	129.8	124.4	
C	3.4828	-1.3691	1.4553	-4.7	13.1	162.5	57.0	158.3	0.17	129.7	124.3	
C	3.4828	-1.3691	-1.4553	-4.7	13.1	162.5	57.0	158.3	0.17	129.7	124.3	
Th	-0.0834	-1.7442	0.0000									

Th@C₈₆

	X	Y	Z	σ_{11}	σ_{22}	σ_{33}	σ_{iso}	σ_{anis}	σ_{asym}	δ vs TMS	δ vs C ₆₀	Average per type
C	-4.2141	1.1330	0.3746	-47.4	-24.8	143.0	23.6	179.1	0.19	163.1	157.7	157.7
C	-0.5952	-1.2079	4.1117	-57.5	-20.0	158.8	27.1	197.5	0.28	159.6	154.2	154.2
C	-2.8658	2.5568	1.8108	-30.7	-27.6	142.2	28.0	171.4	0.03	158.7	153.3	153.3
C	-3.1893	1.4228	-3.0214	-46.2	-21.7	154.9	29.0	188.9	0.19	157.7	152.3	152.3
C	-3.4097	0.2911	2.5040	-35.5	-18.9	143.3	29.6	170.5	0.15	157.1	151.7	151.7
C	-2.9039	-1.0021	-3.3663	-42.4	-28.6	160.4	29.8	195.9	0.11	156.9	151.5	151.5
C	-3.7347	-1.2553	-2.2095	-45.6	-17.2	153.1	30.1	184.5	0.23	156.6	151.2	151.2
C	-1.7790	2.5816	2.7564	-45.5	-7.8	153.1	33.2	179.7	0.31	153.4	148.0	148.0
C	-2.6212	0.3142	-3.7610	-45.7	-7.0	154.1	33.8	180.4	0.32	152.9	147.5	147.5
C	2.1074	3.6624	-0.7105	-42.1	-12.9	157.7	34.2	185.2	0.24	152.5	147.1	147.1
C	3.1945	2.0176	2.2640	-43.7	-10.4	156.7	34.2	183.7	0.27	152.4	147.1	
C	-2.3681	0.3477	3.4982	-34.7	-15.7	155.4	35.0	180.6	0.16	151.7	146.3	146.3
C	0.3066	-0.0937	4.3162	-29.1	-22.3	156.7	35.1	182.4	0.06	151.6	146.2	146.2
C	-3.9142	1.9854	-0.7542	-30.1	-22.5	158.1	35.2	184.4	0.06	151.5	146.1	
C	-4.0213	1.1798	-1.9335	-45.9	0.0	153.9	36.0	176.9	0.39	150.7	145.3	145.3
C	0.3709	3.4814	-2.4241	-23.0	-21.0	156.6	37.5	178.7	0.02	149.2	143.8	143.8
C	-2.4919	3.3447	0.6690	-26.3	-18.9	158.5	37.8	181.1	0.06	148.9	143.5	143.5
C	2.8160	3.0111	1.3788	-46.8	5.8	155.3	38.1	175.8	0.45	148.6	143.2	143.2
C	-1.8885	-0.9848	3.6745	-49.1	11.9	151.7	38.2	170.4	0.54	148.5	143.1	
C	-1.2808	0.6776	-4.1455	-30.7	-11.4	156.9	38.3	177.9	0.16	148.4	143.0	143.0
C	-0.7498	3.4188	2.2150	-26.8	-11.9	153.6	38.3	173.0	0.13	148.4	143.0	
C	-1.0899	2.0534	-3.7453	-46.4	10.9	150.6	38.3	168.4	0.51	148.3	143.0	
C	1.5451	3.6691	1.5377	-24.0	-14.7	154.0	38.4	173.4	0.08	148.2	142.9	142.8
C	-1.8582	-1.9718	-3.3848	-32.9	-5.8	154.2	38.5	173.6	0.23	148.2	142.8	

C	3.8998	0.8712	1.7724	-31.4	-4.0	150.9	38.5	168.6	0.24	148.2	142.8	
C	2.3121	1.6118	3.3371	-28.0	-16.4	159.9	38.5	182.0	0.10	148.2	142.8	
C	3.1192	2.9027	-0.0266	-28.4	-13.2	158.7	39.0	179.4	0.13	147.6	142.2	142.2
C	-4.3005	-0.1897	-1.5212	-37.7	-2.4	157.4	39.1	177.4	0.30	147.5	142.2	
C	1.7360	3.3222	-1.9933	-33.8	0.3	152.0	39.5	168.7	0.30	147.2	141.8	141.8
C	-3.4753	-1.0523	1.9884	-26.2	-11.7	159.1	40.4	178.0	0.12	146.3	140.9	140.9
C	-2.2073	2.4835	-2.9467	-22.7	-11.9	156.7	40.7	174.0	0.09	146.0	140.6	140.6
C	1.1094	4.0995	0.2304	-24.0	-6.2	152.9	40.9	168.0	0.16	145.8	140.4	140.4
C	2.5261	-2.9938	-2.2678	-18.5	8.3	133.6	41.1	138.7	0.29	145.6	140.2	140.2
C	1.5480	-1.9680	3.6294	-38.8	15.8	146.8	41.3	158.2	0.52	145.4	140.0	140.0
C	-1.1853	3.8773	0.9181	-18.5	-11.2	153.5	41.3	168.4	0.07	145.4	140.0	
C	3.5559	-2.4990	-1.3866	-9.0	-5.4	138.8	41.5	145.9	0.04	145.2	139.8	139.8
C	-1.4675	1.4620	3.5696	-27.4	-2.7	155.8	41.9	170.9	0.22	144.7	139.4	139.4
C	2.6213	0.2381	3.6161	-30.1	-0.1	157.5	42.4	172.6	0.26	144.3	138.9	138.9
C	-0.6710	3.7964	-1.5056	-19.4	-11.2	158.3	42.6	173.7	0.07	144.1	138.7	138.6
C	-2.4915	-1.8365	2.6691	-28.1	-2.3	158.4	42.7	173.6	0.22	144.0	138.6	
C	3.5744	-0.2481	2.6420	-28.0	4.8	151.5	42.8	163.1	0.30	143.9	138.5	
C	0.1721	2.5233	-3.4722	-37.6	11.2	155.4	43.0	168.6	0.43	143.7	138.3	138.2
C	-3.1608	-2.3642	-1.4778	-23.5	-8.2	161.2	43.2	177.0	0.13	143.5	138.1	
C	0.1350	-2.3245	3.6105	-33.1	15.1	148.4	43.5	157.4	0.46	143.2	137.8	137.8
C	-0.0641	1.2301	3.9414	-18.8	-12.7	162.2	43.6	177.9	0.05	143.1	137.7	
C	-2.9274	3.0180	-0.6440	-20.2	-7.1	159.0	43.9	172.6	0.11	142.8	137.4	137.4
C	1.6316	-0.6035	4.0990	-32.1	5.1	158.7	43.9	172.2	0.32	142.8	137.4	
C	0.9829	2.1154	3.4231	-21.3	-7.7	162.3	44.4	176.9	0.12	142.2	136.8	136.7
C	1.5000	-4.3046	-0.3554	-3.8	2.3	135.8	44.8	136.5	0.07	141.9	136.5	
C	1.3120	1.6340	-3.5273	-17.3	-1.0	154.5	45.4	163.7	0.15	141.3	135.9	135.9
C	1.5085	-3.9197	-1.7560	-10.8	9.5	138.5	45.7	139.2	0.22	140.9	135.5	135.5
C	2.5682	-3.8483	0.5197	-10.9	12.8	136.7	46.2	135.8	0.26	140.5	135.1	134.9
C	2.4626	-2.4625	2.6816	-15.2	1.4	153.0	46.4	159.9	0.16	140.3	134.9	
C	-4.3766	-0.2238	-0.0966	-18.7	-0.2	158.1	46.4	167.5	0.17	140.2	134.9	
C	2.2930	2.1394	-2.6100	-19.7	5.9	154.4	46.9	161.3	0.24	139.8	134.4	134.4
C	-3.8323	-1.3191	0.6467	-25.0	1.3	164.4	46.9	176.3	0.22	139.8	134.4	
C	0.4945	-2.4595	-3.2647	-10.0	0.0	150.8	46.9	155.9	0.10	139.8	134.4	
C	0.5508	-3.7305	1.6987	-7.8	-1.6	151.7	47.4	156.4	0.06	139.3	133.9	133.8
C	3.5067	-1.5712	2.1661	-16.5	6.7	152.5	47.6	157.4	0.22	139.1	133.7	
C	-3.6758	1.3979	1.6571	-16.8	-10.7	171.6	48.0	185.3	0.05	138.6	133.3	
C	-2.0113	3.2575	-1.7663	-10.1	-2.1	158.2	48.6	164.3	0.07	138.0	132.7	132.6
C	-0.2045	-0.2434	-4.0912	-9.7	-5.1	160.9	48.7	168.3	0.04	138.0	132.6	
C	0.6181	3.2126	2.5190	-22.5	3.6	165.4	48.8	174.9	0.22	137.8	132.5	
C	3.6304	1.6966	-0.5692	-18.5	4.0	161.6	49.0	168.8	0.20	137.7	132.3	132.3
C	-2.0710	-2.8737	-2.2551	-36.6	30.5	155.0	49.6	158.0	0.64	137.0	131.7	131.7
C	-0.2674	4.1194	-0.1350	-17.9	2.8	164.3	49.7	171.9	0.18	136.9	131.6	131.6

C	3.6074	-2.9478	-0.0028	-3.9	18.7	134.6	49.8	127.2	0.27	136.9	131.5	131.5
C	4.1377	-0.6661	-0.0712	-6.7	5.5	152.5	50.4	153.1	0.12	136.3	130.9	130.9
C	1.9697	-3.4839	1.7825	-7.8	28.3	137.7	52.7	127.4	0.42	134.0	128.6	128.6
C	-1.0274	-3.7686	-0.2203	-5.6	5.5	159.9	53.3	159.9	0.10	133.4	128.0	128.0
C	1.1471	0.2501	-3.7653	-4.4	-0.8	167.6	54.1	170.2	0.03	132.5	127.1	127.1
C	-1.7279	-2.8219	2.0052	-15.8	13.6	164.9	54.2	166.0	0.27	132.4	127.0	127.0
C	1.8531	-2.0416	-3.1199	-5.7	21.4	147.4	54.4	139.5	0.29	132.3	126.9	126.9
C	4.0729	0.6852	0.3770	-4.5	0.0	170.4	55.3	172.7	0.04	131.4	126.0	126.0
C	-0.4003	-3.0999	2.5447	-7.0	6.5	166.5	55.3	166.8	0.12	131.3	125.9	125.9
C	3.1757	1.2818	-1.9059	-5.2	3.9	168.1	55.6	168.8	0.08	131.1	125.7	125.7
C	-1.0280	-3.5879	-1.6598	-11.1	15.1	163.9	56.0	161.9	0.24	130.7	125.3	125.2
C	-0.5396	-1.6175	-3.7572	-4.8	1.6	171.5	56.1	173.1	0.06	130.6	125.2	
C	2.1605	-0.6241	-3.2071	5.1	7.4	155.8	56.1	149.5	0.02	130.6	125.2	
C	-2.0281	-3.1101	0.5981	-4.9	7.9	166.3	56.4	164.9	0.12	130.2	124.9	124.9
C	3.1669	-0.1154	-2.2953	1.2	10.6	157.5	56.4	151.7	0.09	130.2	124.9	
C	-3.1262	-2.3917	-0.0567	-2.3	8.4	163.7	56.6	160.7	0.10	130.1	124.7	124.7
C	3.9404	-1.7935	0.8033	4.7	21.8	144.6	57.0	131.3	0.19	129.7	124.3	124.3
C	0.2565	-3.5311	-2.3362	1.1	25.4	148.5	58.3	135.3	0.27	128.4	123.0	123.0
C	0.2397	-4.1537	0.3697	3.2	23.0	150.3	58.8	137.2	0.22	127.8	122.4	122.4
C	3.8059	-1.0684	-1.4046	4.9	27.6	149.8	60.8	133.6	0.26	125.9	120.5	120.5

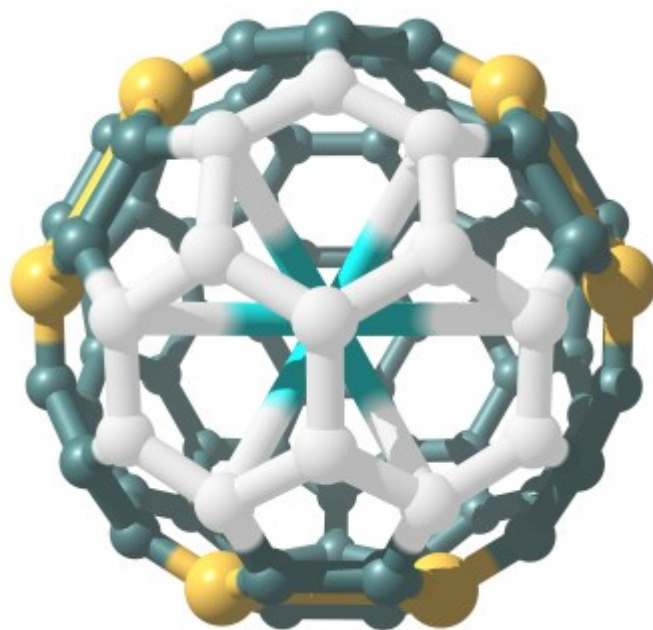


Figure S1. Most shielded carbon atoms calculated at 124.4 ppm (Exp. 128.5 ppm), in yellow for Th@C₈₂. Three-fused six-membered rings motif coordinating Th is given in white.

Table S2. Energy decomposition analysis for the Th-Fullerene interaction. Values in kcal mol⁻¹.

	Th@C ₇₆		Th@C ₈₀		Th@C ₈₂		Th@C ₈₆		Average*
ΔE_{Pauli}	870.9		816.1		822.3		904.8		
ΔE_{Estat}	-509.9	47.6%	-487.6	47.9%	-487.1	46.6%	-527.4	48.0%	47.5%
ΔE_{Orb}	-550.2	51.4%	-524.6	51.5%	-547.0	52.3%	-562.9	51.2%	51.6%
ΔE_{Disp}	-11.1	1.0%	-6.4	0.6%	-11.9	1.1%	-9.5	0.9%	0.9%
ΔE_{int}	-200.3		-202.4		-223.7		-195.0		

*Average depicted at the main text.

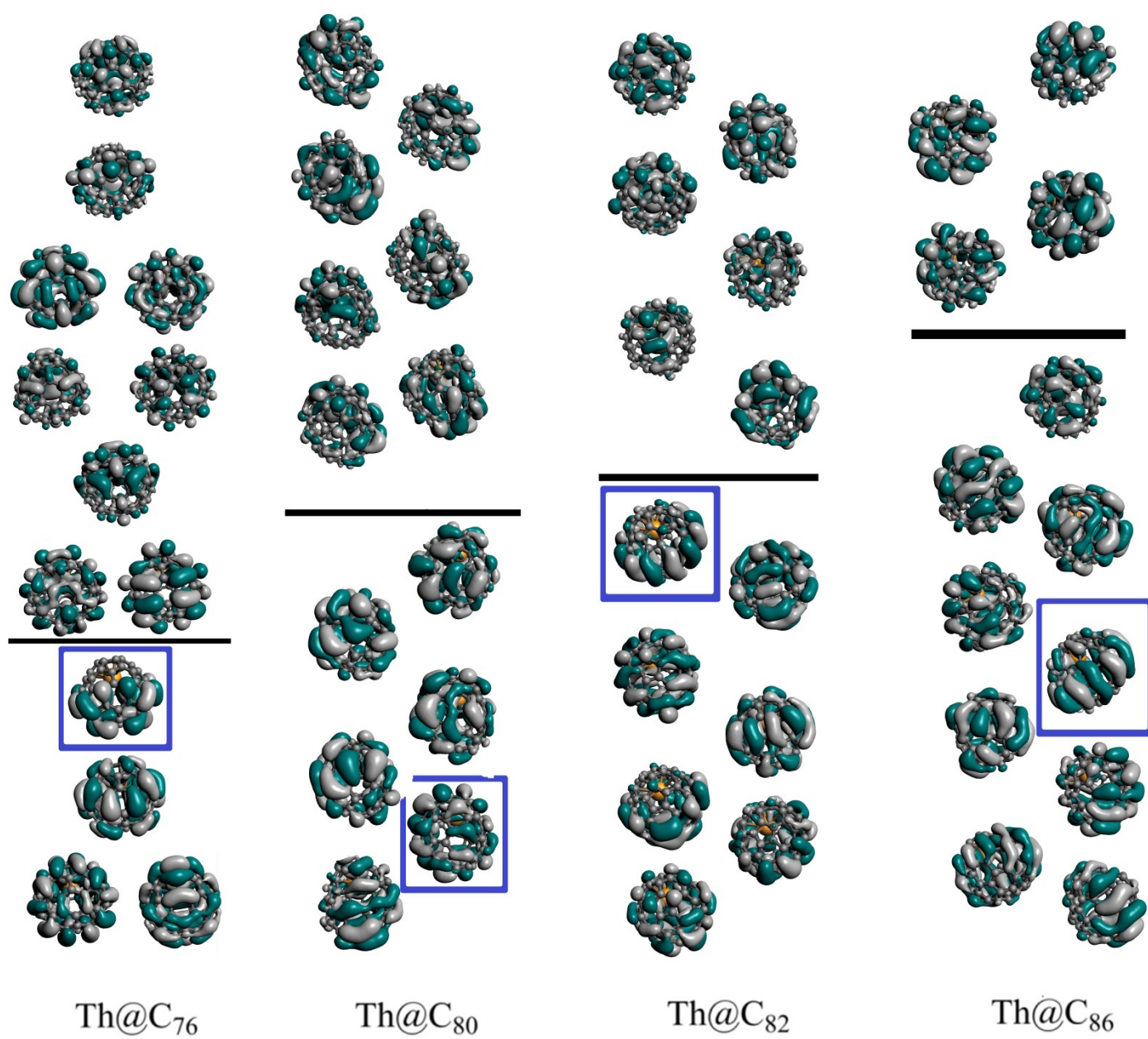


Figure S2. Frontier molecular orbitals for the studied series depicting the I-shell. Blue boxes denote MOs given at Figure 4 from the main document. Black lines shows the HOMO (below) and LUMO (above) limit.