Exaltation of polarizability as a common property of fullerene dimers with diverse intercage bridges

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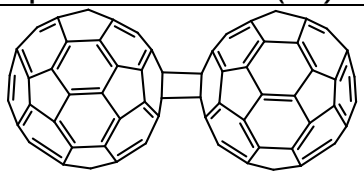
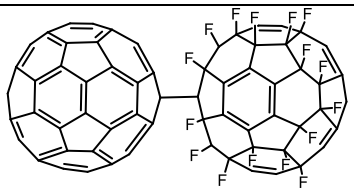
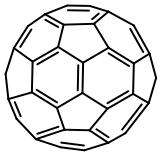
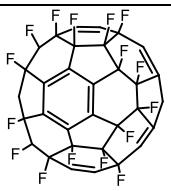
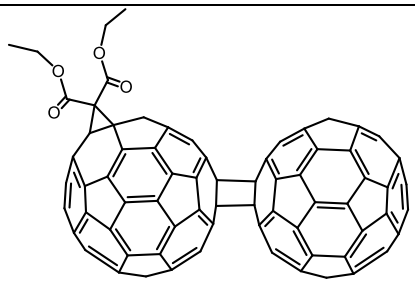
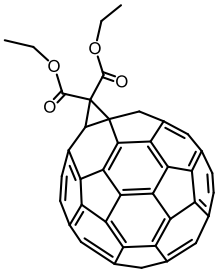
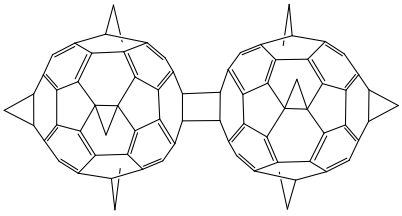
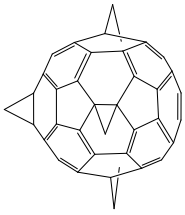
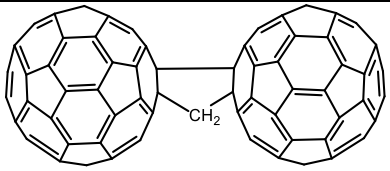
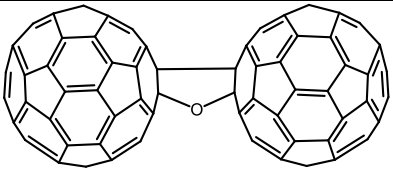
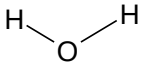
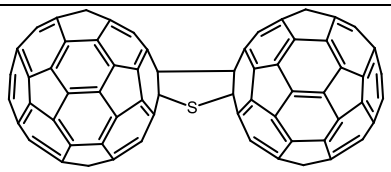
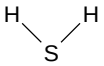
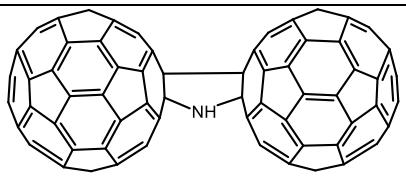
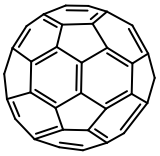
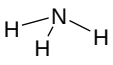
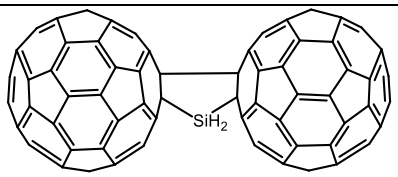
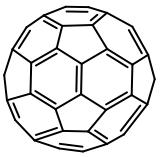
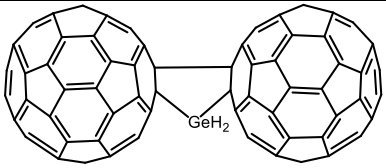
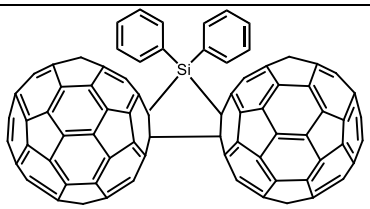
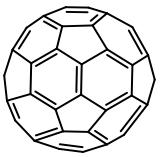
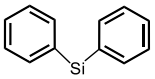
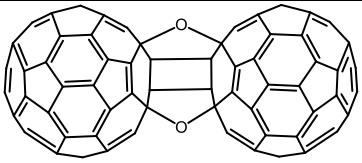
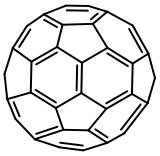
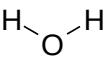
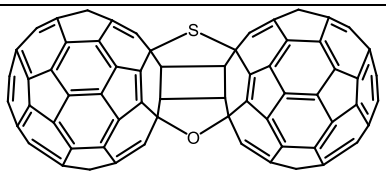
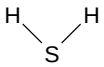
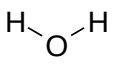
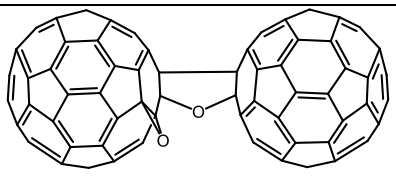
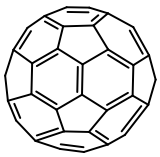
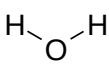
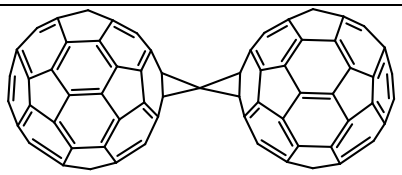
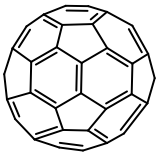
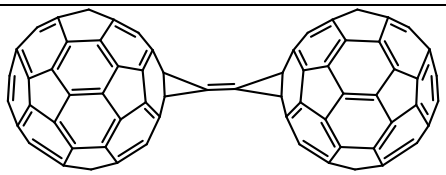
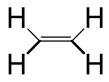
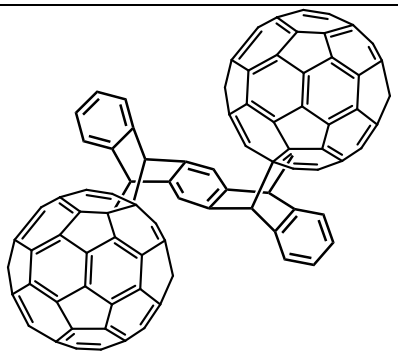
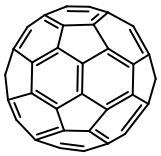
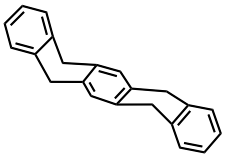
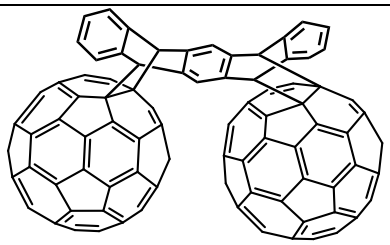
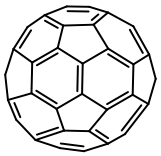
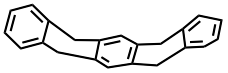
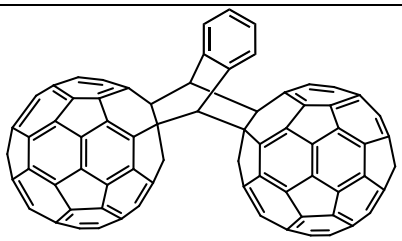
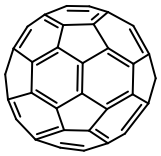
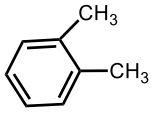
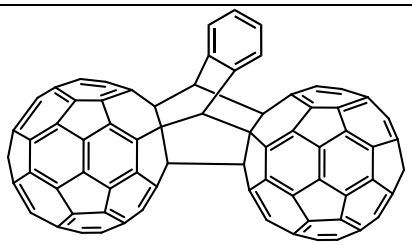
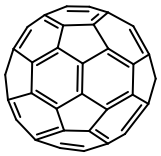
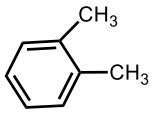
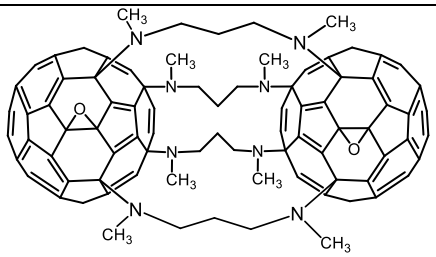
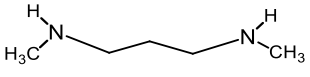
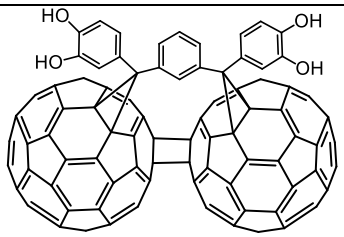
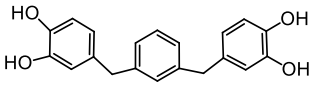
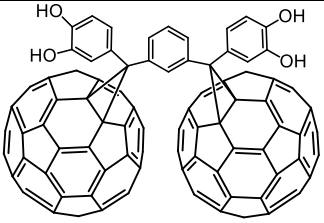
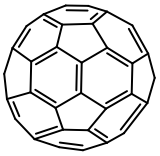
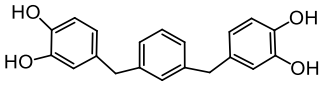
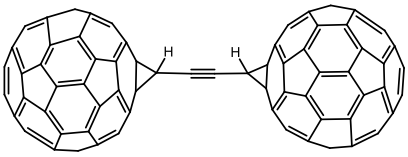
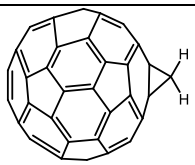
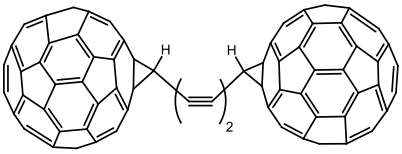
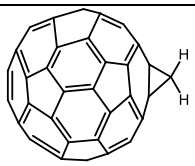
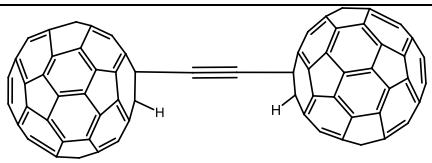
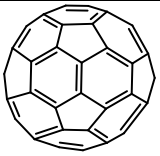
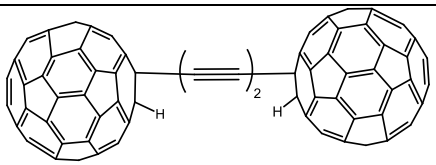
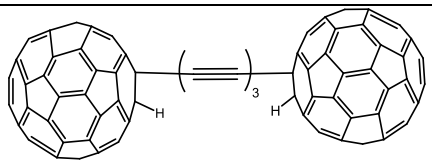
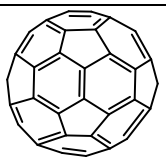
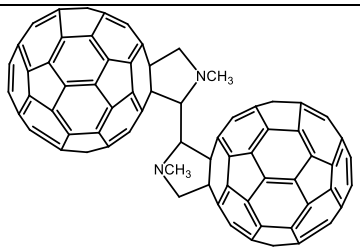
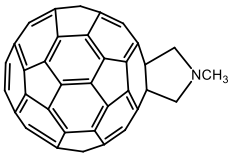
SUPPLEMENTARY MATERIALS

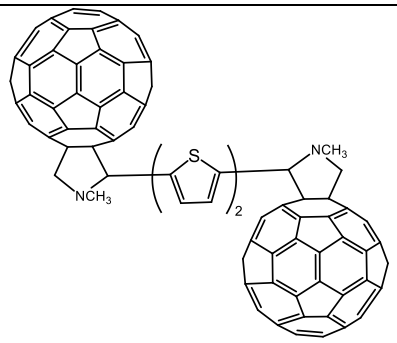
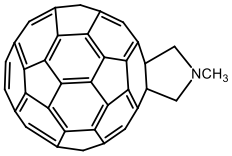
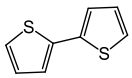
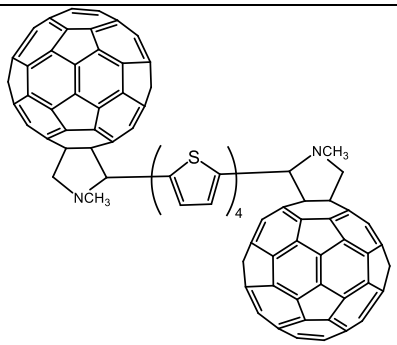
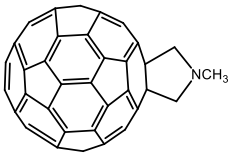
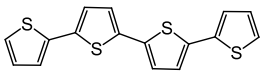
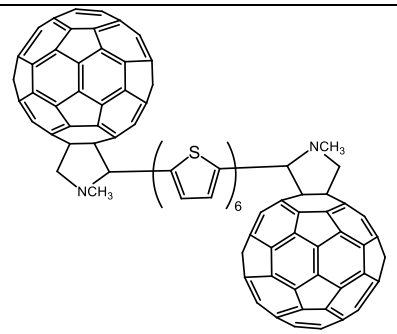
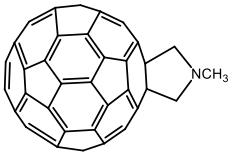
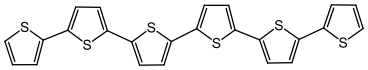
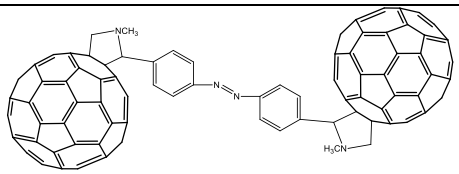
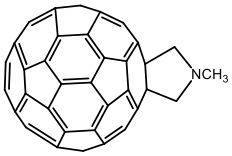
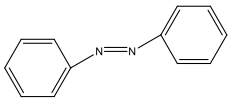
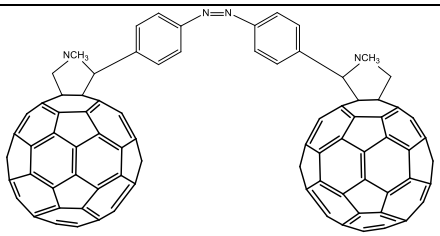
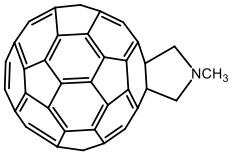
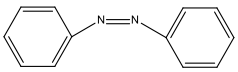
The table below represents the mean polarizabilities of the studied fullerene dimers and the relevant one-cage compounds required for calculations within the additive scheme used in the work. All values have been calculated with the PBE/3ζ density functional theory method in terms of the finite field approach.

#	Dimers and their polarizabilities (Å^3)	Structural subunits and their polarizabilities (Å^3)	Δα (Å^3)
1	 179.90	2  82.67	14.63
2	 182.96	 82.67 +  87.43	12.86
3	 198.70	 82.67 +  100.00	16.02
4	 199.46	2  93.29	12.87
5	 185.43	2  82.67 + CH_4 2.30	17.78
6	 184.24	2  82.67 +  1.08	17.82

7	 191.76	2  +  82.67 3.02	23.40
8	 185.88	2  +  82.67 1.68	18.86
9	 190.16	2  + SiH_4 82.67 4.58	20.23
10	 191.90	2  + GeH_4 82.67 5.00	21.56
11	 210.65	2  +  82.67 24.82	20.49
12	 181.60	2  + 2  82.67 1.08	14.11
13	 186.20	2  +  +  82.67 3.02 1.08	16.77
14	 183.33	 +  +  82.67 1.08 83.24	15.26
15	 180.94	2  + CH_4 82.67 2.30	13.30

16	 183.96	2  +  82.67 3.75	14.87
17	 214.45	2  +  82.67 38.46	10.64
18	 213.89	2  +  82.67 38.22	10.34
19	 192.70	2  +  82.67 14.00	13.37
20	 193.54	2  +  82.67 14.00	14.21
21	 226.97	2  + 4  83.24 12.60	10.07

22	 214.54	2  +  82.67 37.86	11.33
23	 220.96	2  +  82.67 37.86	17.76
24	 183.60	2  + 85.01 3.02	10.56
25	 192.29	2  + 85.01 6.96	15.32
26	 182.37	2  + 82.67 3.02	14.01
27	 196.16	2  + 82.67 6.96	23.86
28	 213.94	2  + 82.67 12.87	35.74
29	 193.05	2  91.95	9.15

30	 219.53	2  91.95 +  20.44	15.19
31	 272.80	2  91.95 +  55.93	32.98
32	 338.60	2  91.95 +  107.60	47.10
33	 228.44	2  91.95 +  28.38	16.17
34	 224.16	2  91.95 +  24.33	15.93