Supplementary Materials to the article:

Digitalizing Structure–Symmetry Relations at the Formation of Endofullerenes in Terms of Information-Entropy Formalism

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Numerical data on the formation of endofullerenes X@C_{84} associated with Figure 8.

Isomer	Partition	σ	χ	h_{C_N}	$h_{X@C_N}$	H_{reorg}^{str}
C_{84}-1 (D_2)	21×4	4	168	4.392	4.433	0.041
C_{84}-2 (C_2)	42×2	2	84	5.392	5.421	0.029
C_{84}-3 (C_S)	4×1 + 40 ×2	1	80	5.440	5.468	0.028
C_{84}-4 (D_{2d})	3×4 + 9×8	4	240	3.535	3.586	0.051
C_{84}-5 (D_2)	21×4	4	168	4.392	4.433	0.041
C_{84}-6 (C_{2v})	4×2 + 19×4	2	160	4.488	4.527	0.039
C_{84}-7 (C_{2v})	4×2 + 19×4	2	160	4.488	4.527	0.039
C_{84}-8 (C_2)	42×2	2	84	5.392	5.421	0.029
C_{84}-9 (C_2)	42×2	2	84	5.392	5.421	0.029
C_{84}-10 (C_S)	8×1 + 38×2	1	76	5.488	5.515	0.028
C_{84}-11 (C_2)	42×2	2	84	5.392	5.421	0.029
C_{84}-12 (C_1)	84×1	1	0	6.392	6.409	0.017
C_{84}-13 (C_2)	42×2	2	84	5.392	5.421	0.029
C_{84}-14 (C_S)	2×1 + 41×2	1	82	5.416	5.445	0.029
C_{84}-15 (C_S)	4×1 + 40×2	1	80	5.440	5.468	0.028
C_{84}-16 (C_S)	2×1 + 41×2	1	82	5.416	5.445	0.029
C_{84}-17 (C_{2v})	6×2 + 18×4	2	156	4.535	4.574	0.039
C_{84}-18 (C_{2v})	2×2 + 20×4	2	164	4.440	4.480	0.040
C_{84}-19 (D_{3d})	2×6 + 6×12	6	289	2.950	3.008	0.058
C_{84}-20 (T_d)	1×12 + 3×24	12	373	1.950	2.020	0.069
C_{84}-21 (D_2)	21 ×4	4	168	4.392	4.433	0.041
C_{84}-22 (D_2)	21×4	4	168	4.392	4.433	0.041
C_{84}-23 (D_{2d})	1×4 + 10×8	4	248	3.440	3.492	0.052
C_{84}-24 (D_{6h})	3×12 + 2×24	12	349	2.236	2.302	0.066