Supporting Information

A Theoretical Study on the Strain Energy of Carbon Nanobelts

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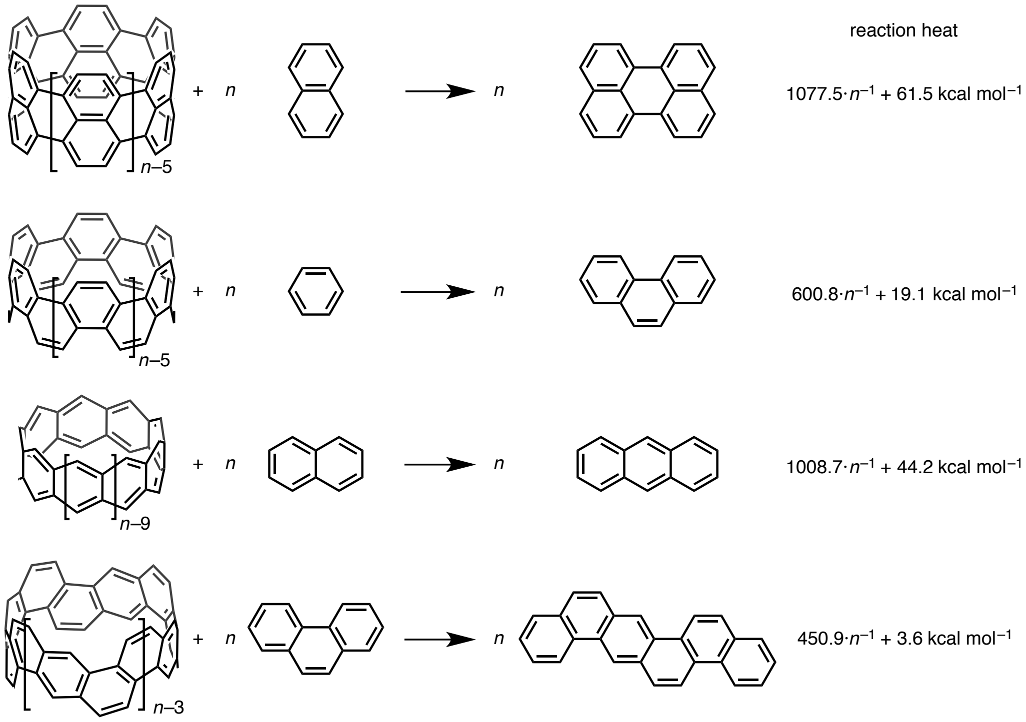
1. Hypothetical reactions

Scheme S1. Hypothetical reactions for carbon nanobelts (additional unsuccessful results).



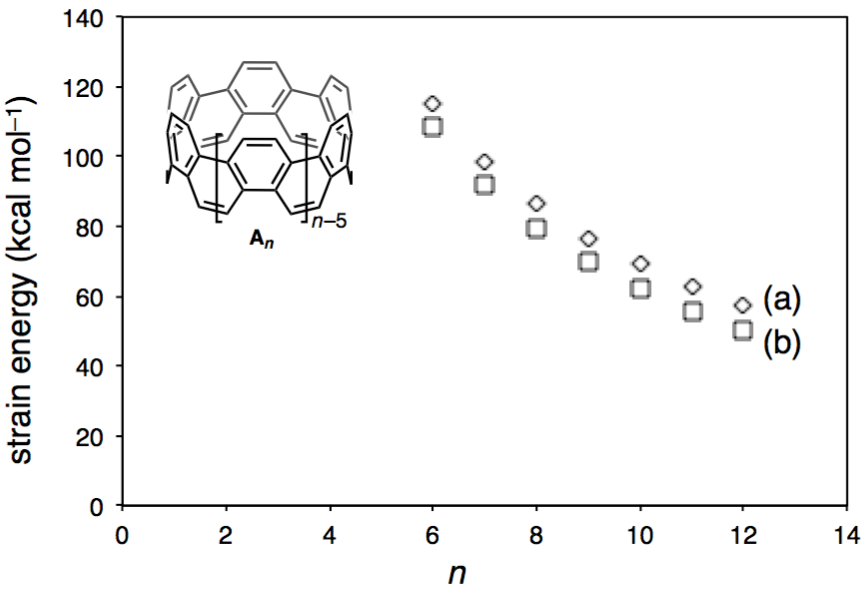
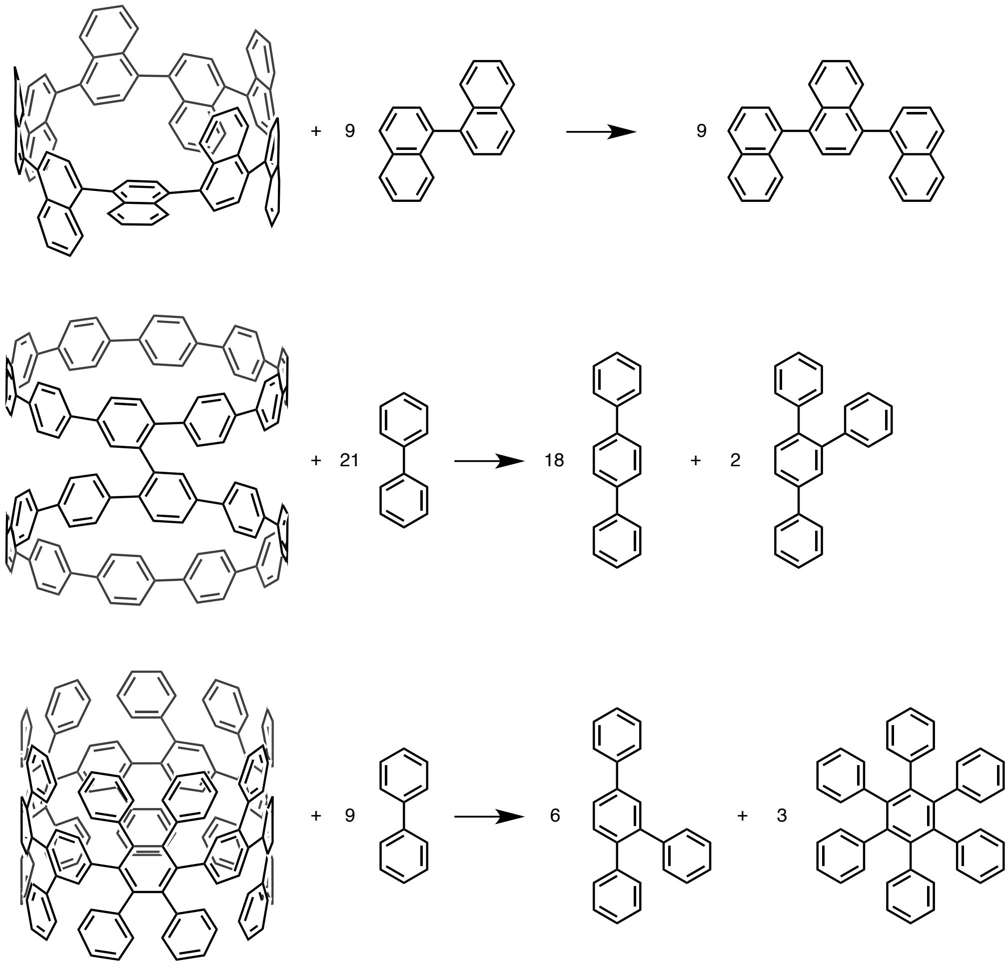


Figure S1. Strain energy of $\mathbf{A}_n$ obtained from the current method shown in Figure 4 (a) and from the unsuccessful hypothetical reaction shown in eq 2 (b).

Scheme S2. Hypothetical homodesmotic reactions for the possible precursors for CNBs



2. POAV analysis

Table S1. POAV angles of [*n*]CPP, $\mathbf{A}_n$, and $\mathbf{B}_n$ (°)

n	[*n*]CPP	$\mathbf{A}_n$	$\mathbf{B}_n$
6	3.493 (24C)	2.096 (24C)	1.953 (24C)
	6.101 (12C)	4.548 (24C)	4.405 (24C)
			4.185 (12C)
8	2.821 (32C)	1.603 (32C)	1.547 (32C)
	4.633 (16C)	3.245 (32C)	3.147 (32C)
			2.759 (16C)
10	2.403 (40C)	1.278 (40C)	1.271 (40C)
	3.747 (20C)	2.424 (40C)	2.414 (40C)
			2.001 (20C)
12	2.109 (48C)	1.083 (48C)	1.066 (48C)
	3.126 (24C)	2.087 (48C)	1.955 (48C)
			1.537 (24C)

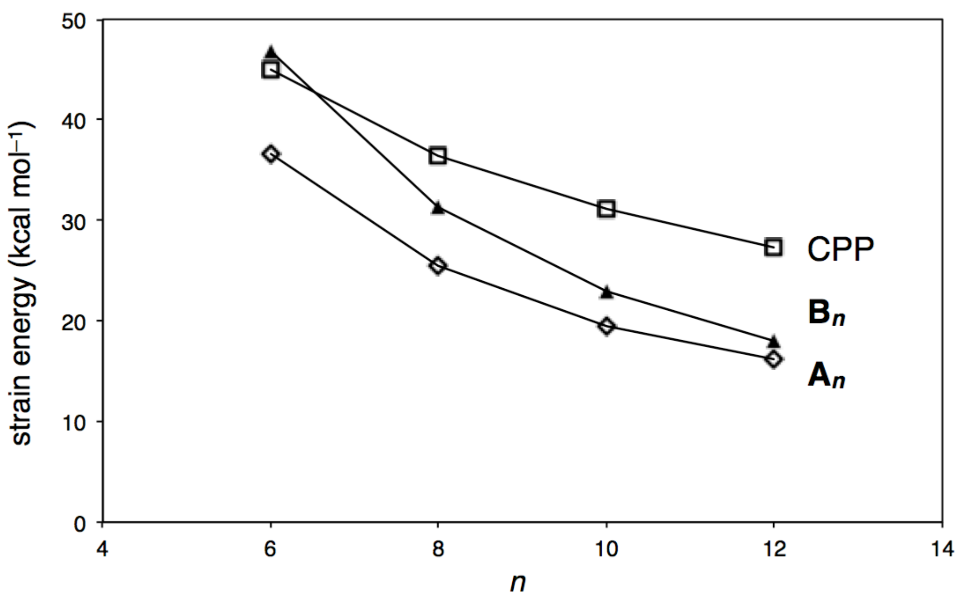


Figure S2. Strain energies of [*n*]CPP, $\mathbf{A}_n$, and $\mathbf{B}_n$ calculated by using $\Sigma(\theta_{\sigma\pi}-1/2\pi)^2 \times 200$ (kcal/mol).

3. Plot for strain energies of CNBs

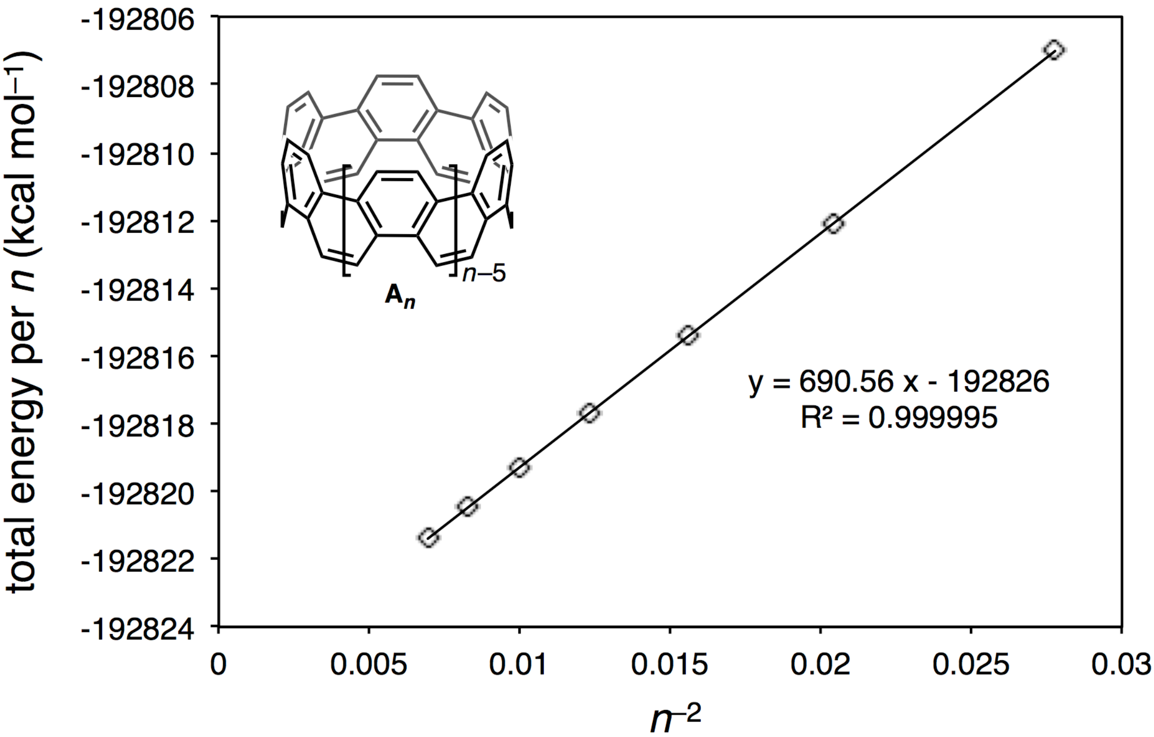


Figure S3. Plot of the total energy per n of $\mathbf{A}_n$ as a function of n^{-2} with the linear regulation line.

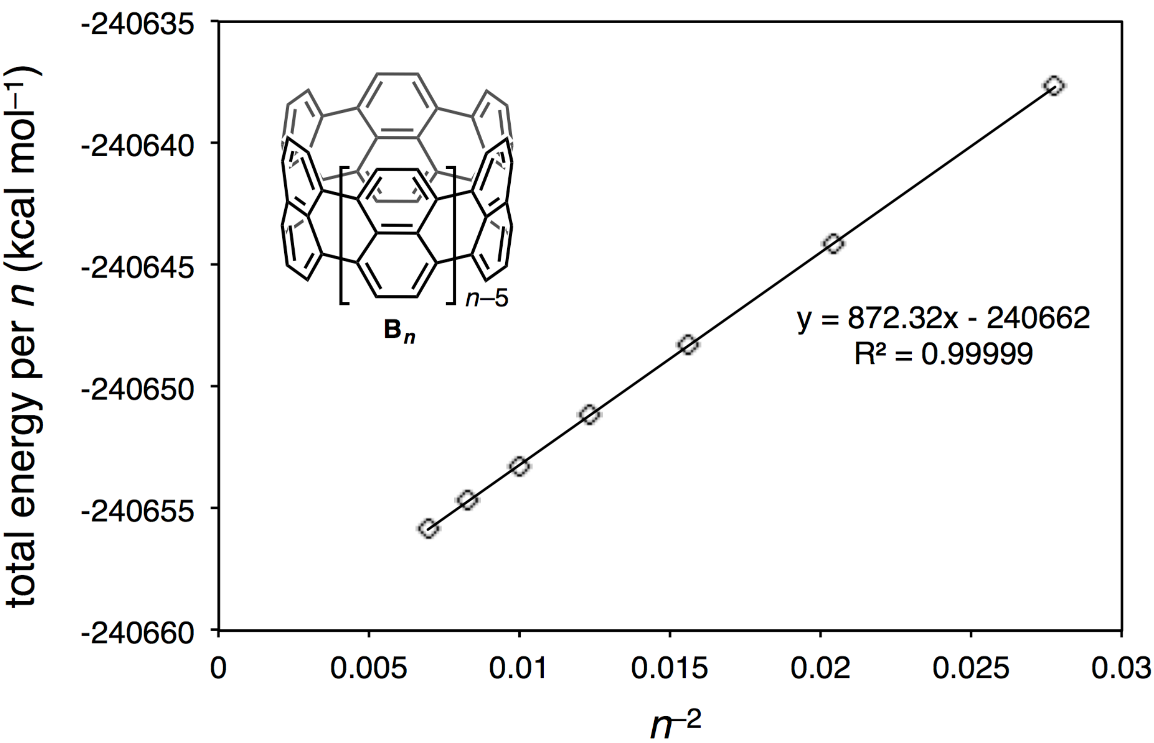


Figure S4. Plot of the total energy per n of $\mathbf{B}_n$ as a function of n^{-2} with the linear regulation line.

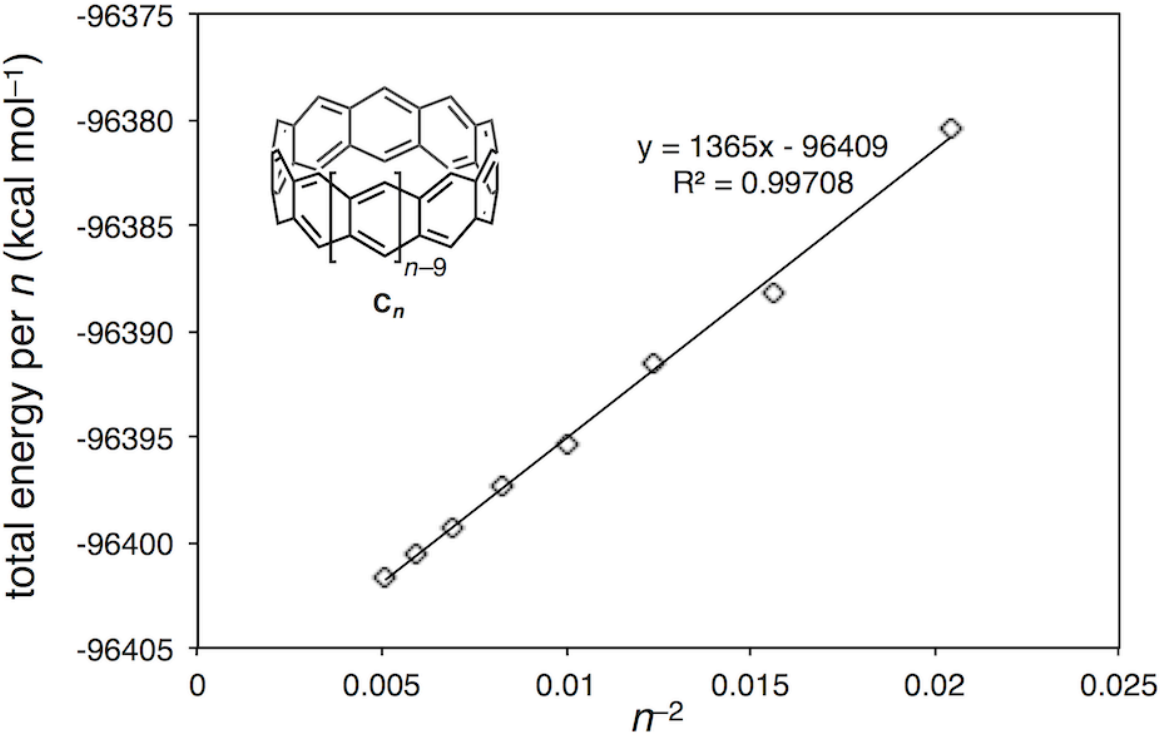


Figure S5. Plot of the total energy per n of $\mathbf{C}_n$ as a function of n^{-2} with the linear regulation line.

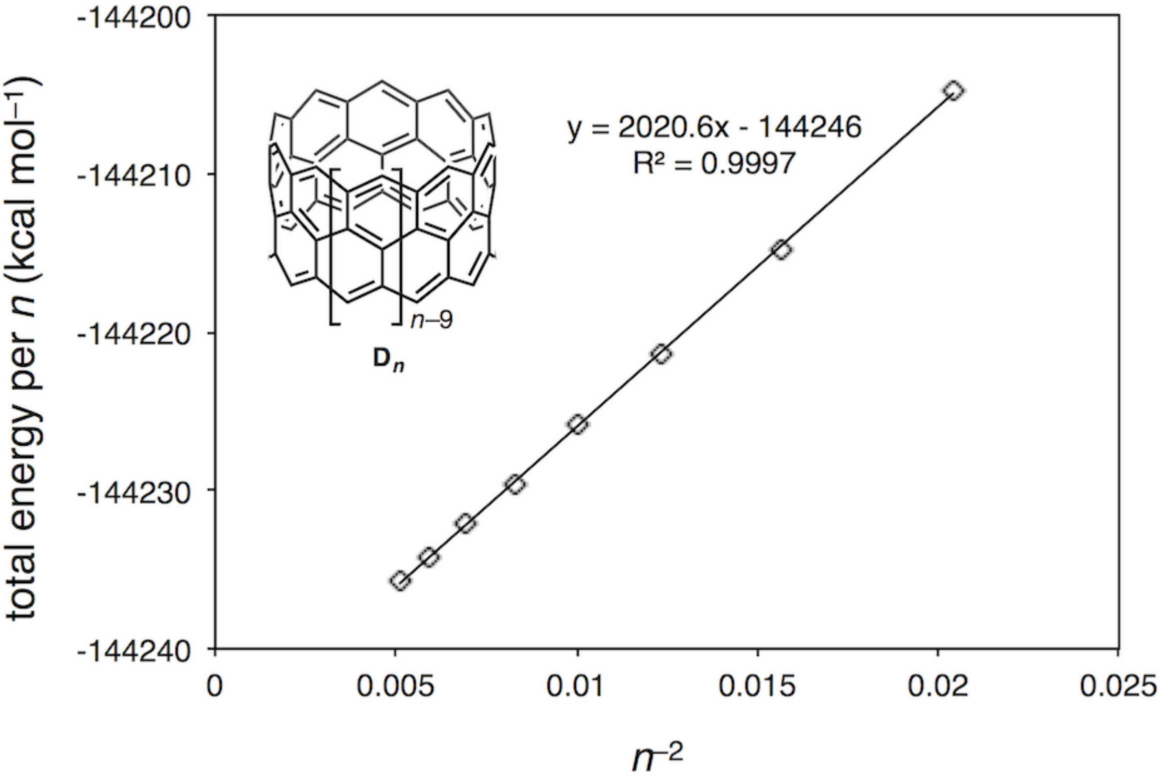


Figure S6. Plot of the total energy per n of $\mathbf{D}_n$ as a function of n^{-2} with the linear regulation line.

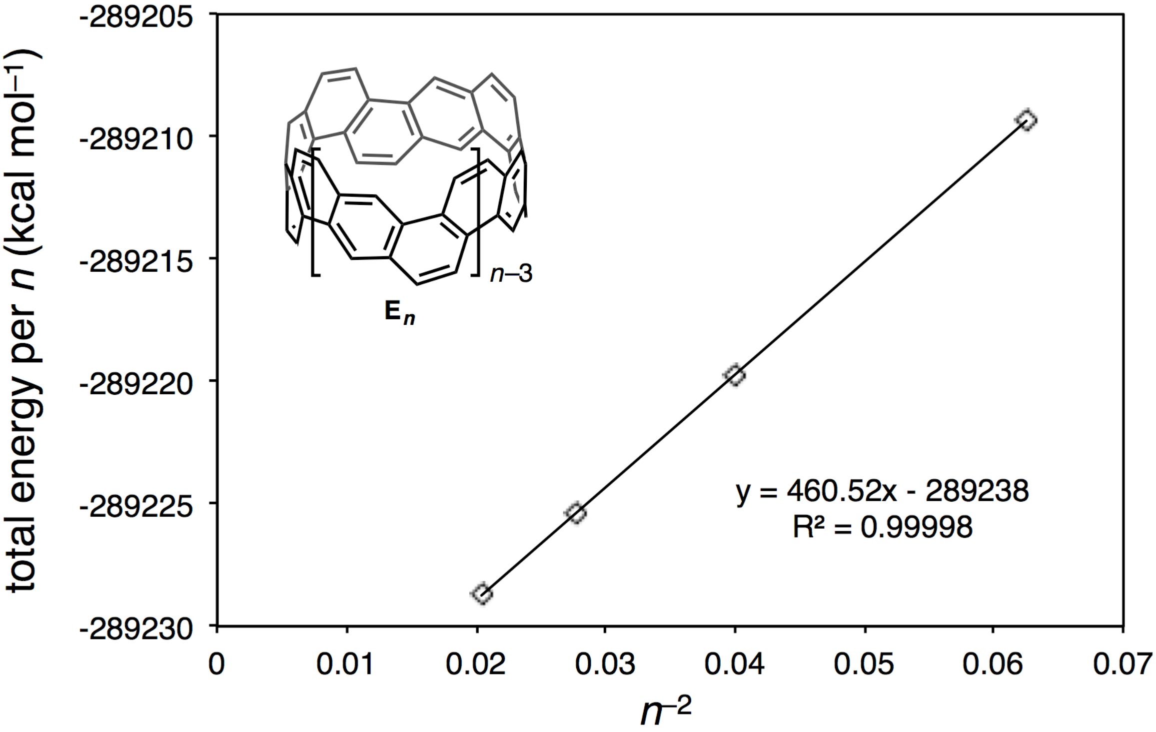


Figure S7. Plot of the total energy per n of $\mathbf{E}_n$ as a function of n^{-2} with the linear regulation line.

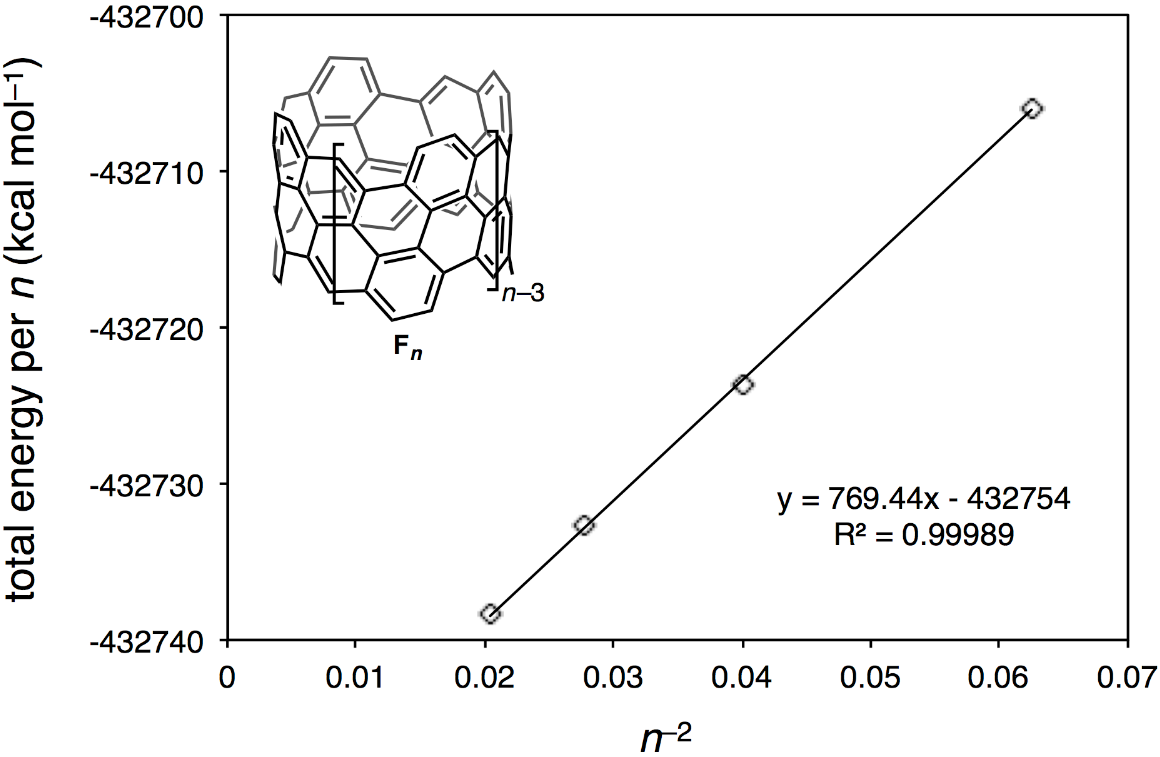


Figure S8. Plot of the total energy per n of $\mathbf{F}_n$ as a function of n^{-2} with the linear regulation line.

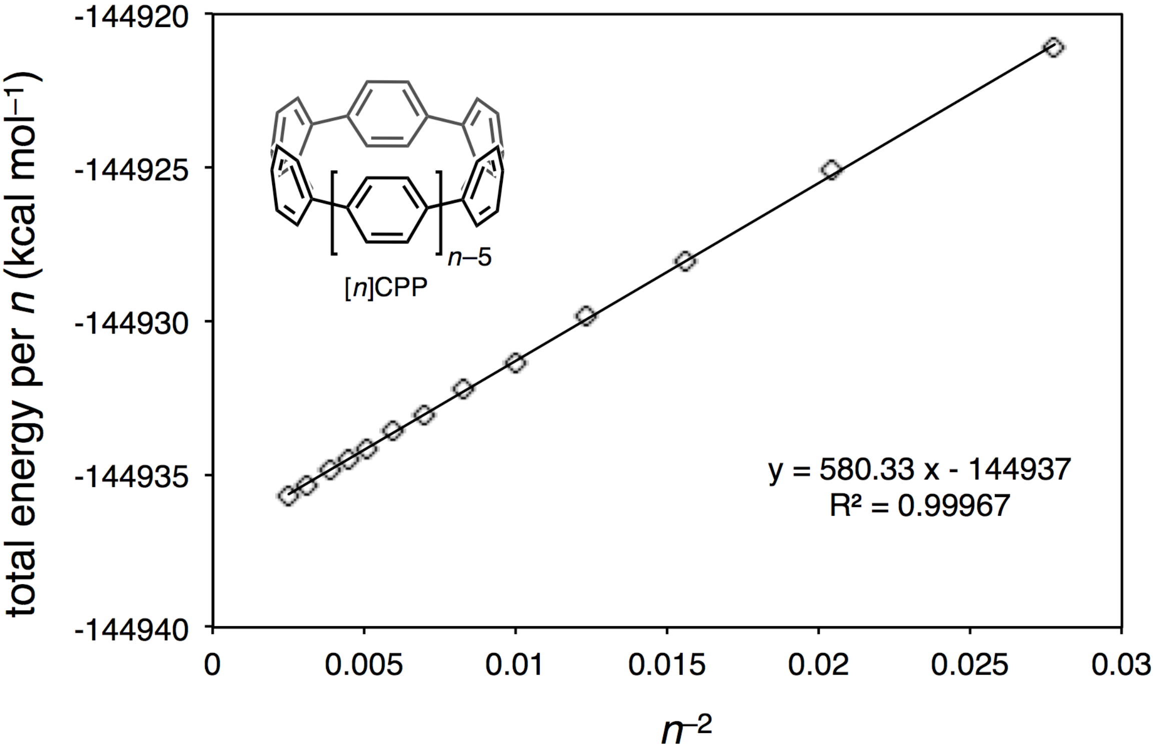


Figure S9. Plot of the total energy per *n* of [*n*]CPP as a function of n^{-2} with the linear regulation line.

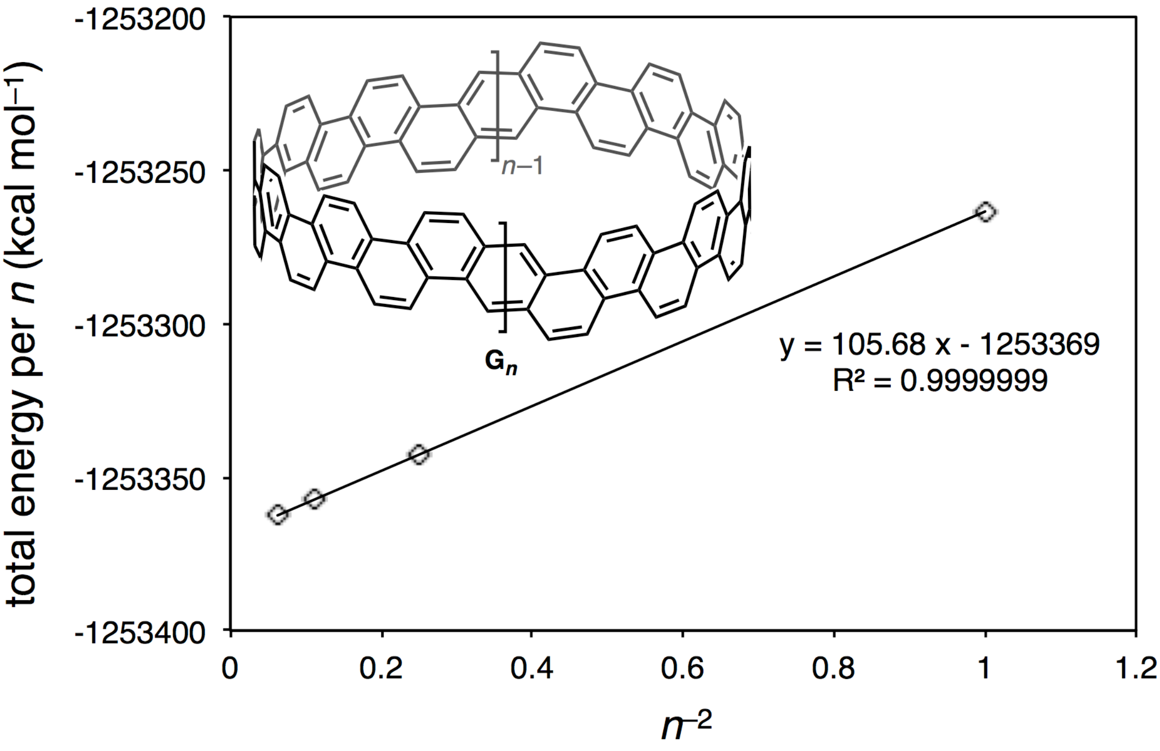


Figure S10. Plot of the total energy per *n* of $\mathbf{G}_n$ as a function of n^{-2} with the linear regulation line.

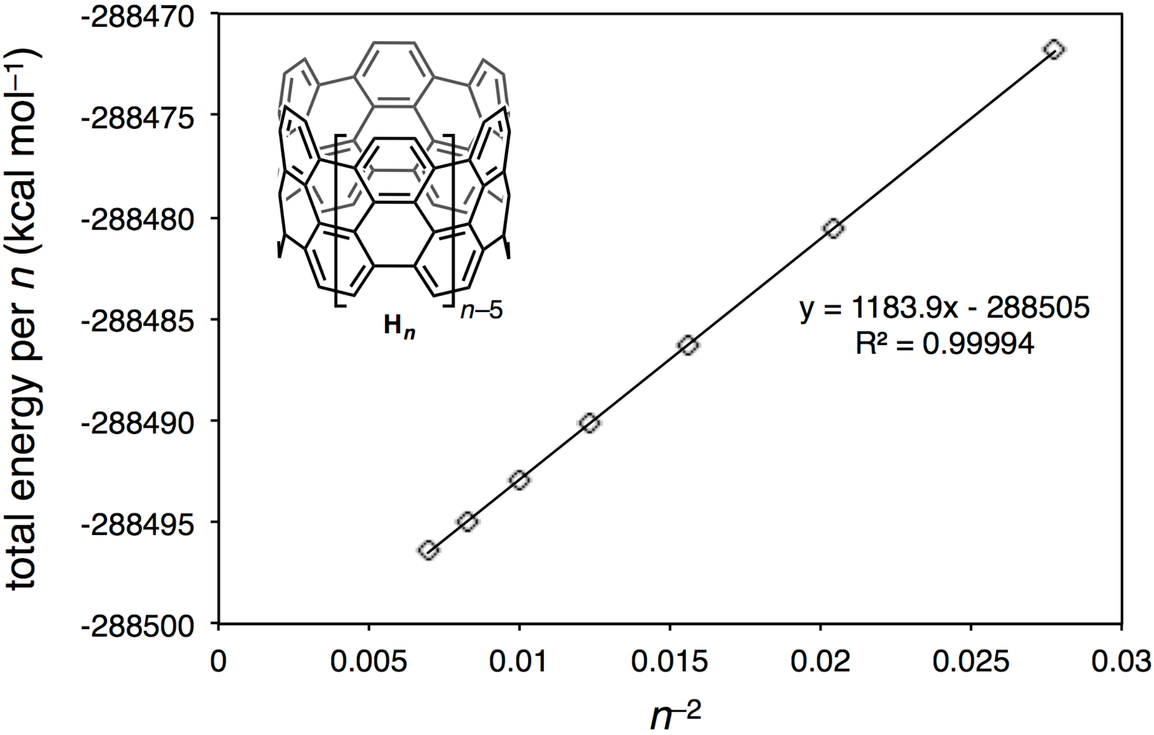


Figure S11. Plot of the total energy per n of $\mathbf{H}_n$ as a function of n^{-2} with the linear regulation line.

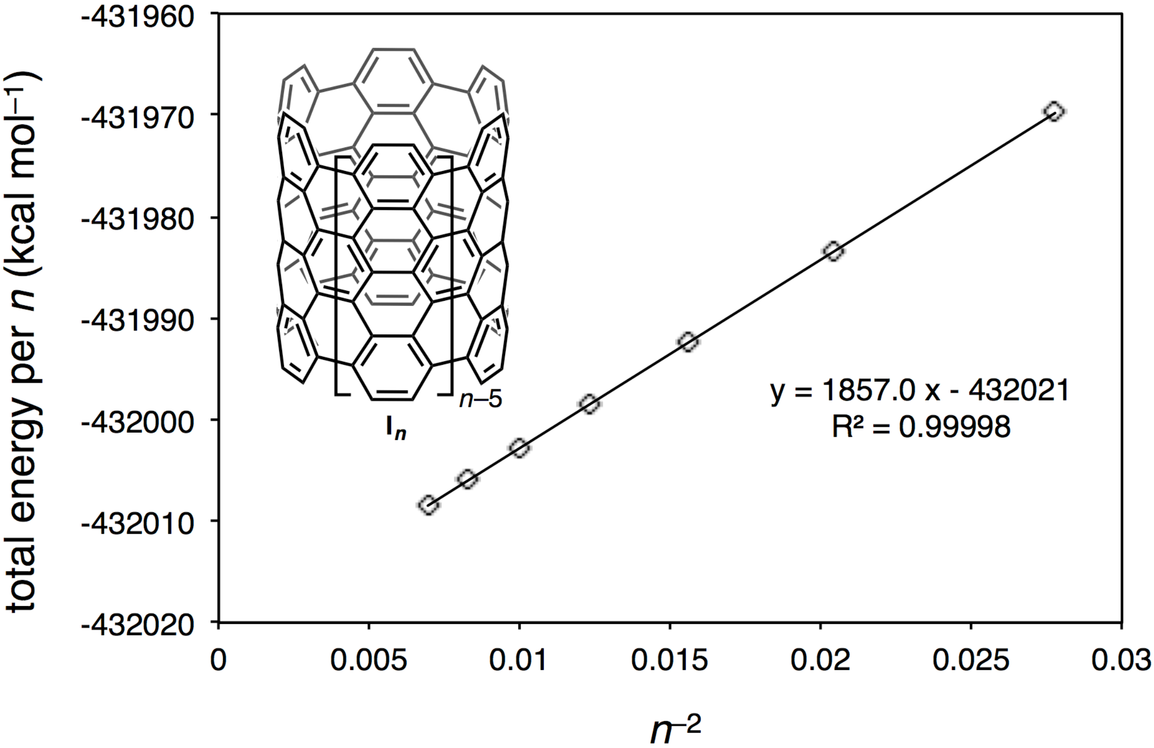


Figure S12. Plot of the total energy per n of $\mathbf{I}_n$ as a function of n^{-2} with the linear regulation line.

4. Complete reference 11a

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, *Revision C.01*, Gaussian, Inc., Wallingford CT, 2010.