

Zigzag and spiral configurations for fullerenes in carbon nanotubes

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Corrigendum

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There is a minor error in equation (A.4) and in the equation following (A.4). The correct form of (A.4) reads,

$$P_n = \frac{4\pi^2 a^2 C_n \eta_f^2}{r(2-n)(3-n)} \left(\frac{1}{(2a+r)^{n-3}} + \frac{1}{(-r)^{n-3}} - \frac{1}{(2a-r)^{n-3}} - \frac{1}{r^{n-3}} \right), \quad (\text{A.4})$$

and for n even the correct simplification of this equation becomes

$$P_n = \frac{4\pi^2 a^2 C_n \eta_f^2}{r(2-n)(3-n)} \left(\frac{1}{(2a+r)^{n-3}} - \frac{1}{(2a-r)^{n-3}} - \frac{2}{r^{n-3}} \right).$$

This change has a small effect on numerical values presented in the original tables 2 and 3. The corrected revised tables 2 and 3 are given below. The authors are grateful to Dr. Barry Cox for pointing out this error.

Table 2. Equilibrium distance Z (Å), offset location ε (Å) and total potential energy of the system E^{tot} (eV) for each pair of C_{60} fullerenes in a zigzag configuration nanopeapod comprising $(2k + 1)$ C_{60} molecules.

k	(10,10)			(16,16)			(20,20)		
	Z	ε	E^{tot}	Z	ε	E^{tot}	Z	ε	E^{tot}
1	10.0550	0	-6.7632	5.2176	4.2977	-2.7048	0	7.0213	-2.0941
2	10.0543	0	-13.8074	5.0390	4.3216	-6.2354	5.0267	7.0220	-4.7420
3	10.0542	0	-20.8516	5.0366	4.3232	-9.7692	5.0269	7.0217	-7.3973
4	10.0542	0	-27.8958	5.0358	4.3239	-13.3031	5.0269	7.0215	-10.0526
5	10.0541	0	-34.9400	5.0354	4.3244	-16.8370	5.0269	7.0214	-12.7079
10	10.0541	0	-70.1612	5.0347	4.3251	-34.5067	5.0270	7.0212	-25.9845
15	10.0540	0	-105.3823	5.0345	4.3255	-52.1764	5.0270	7.0211	-39.2611
20	10.0540	0	-140.6034	5.0344	4.3255	-69.8460	5.0270	7.0211	-52.5377
25	10.0540	0	-175.8245	5.0344	4.3256	-87.5157	5.0270	7.0210	-65.8143
50	10.0540	0	-351.9301	5.0343	4.3257	-175.8641	5.0270	7.0210	-132.1973
100	10.0540	0	-704.1413	5.0342	4.3258	-352.5610	5.0270	7.0210	-274.9634

Table 3. Angular spacing α , longitudinal spacing β , offset location ε in Å and total potential energy of the system E^{tot} (eV) for each pair of C_{60} fullerenes in a spiral configuration nanopеapod comprising k C_{60} molecules.

k	(10,10)			(16,16)			(20,20)					
	α	β	ε	α	β	ε	α	β	ε			
3	0	10.0545	0	-10.2852	3.1416	5.0442	4.3195	-4.4671	1.3490	4.9083	7.0251	-3.6709
4	0	10.0543	0	-13.8075	3.1416	5.0385	4.3216	-6.2395	1.5566	0.8831	7.0239	-5.2978
5	0	10.0543	0	-17.3297	3.1416	5.0366	4.3226	-8.0120	1.5436	2.4984	7.0057	-6.6966
10	0	10.0541	0	-34.9409	3.1416	5.0341	4.3244	-16.8749	1.5565	2.5063	6.9840	-14.9446
15	0	10.0540	0	-52.5521	3.1416	5.0335	4.3249	-25.7379	1.5649	2.5078	6.9709	-23.1989
20	0	10.0540	0	-70.1633	3.1416	5.0333	4.3251	-34.6029	1.7194	2.2931	6.9181	-33.5703
25	0	10.0540	0	-87.7745	3.1416	5.0331	4.3253	-43.4640	1.7194	2.2934	6.9163	-42.5048
50	0	10.0540	0	-175.8306	3.1416	5.0329	4.3256	-87.7791	1.7194	2.2941	6.9126	-87.1785
100	0	10.0539	0	-351.9426	3.1416	5.0327	4.3259	-176.4093	1.7194	2.2944	6.9108	-176.5269