

Supporting information to the article

Activation energies and information entropies of helium penetration through the fullerene walls. Insights into the formation of endofullerenes $nX@C_{60/70}$ ($n = 1$ and 2) from the information entropy approach

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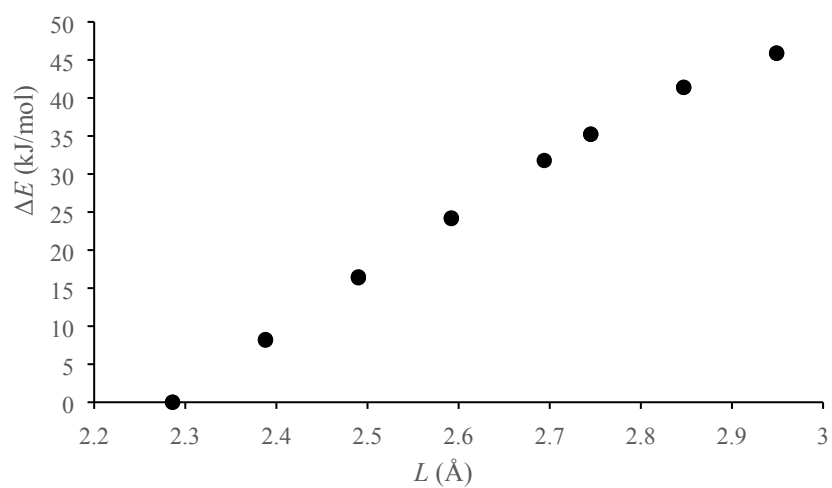
Section A

Structures and imaginary vibration frequencies of the transition states and corresponding activation energies of helium insertion into the fullerenes through the hexagons. The B3LYP/Λ1 calculations*

Transition state	L (Å)	$L_{\text{He}\dots\text{C}}$ (Å)	E_{act} (kJ mol ⁻¹)	ν_{imag} (cm ⁻¹)
TS _{hex} (He + C ₆₀)	1.653 (5.6 bond), 1.500 (6.6 bond)	1.578	843.4	-1148.4
TS _{abccba} (He + C ₇₀)	1.576 (<i>ab</i>), 1.750 (<i>bc</i>), 1.554 (<i>cc</i>), 1.800 (<i>aa</i>)	1.662– 1.678	859.1	-991.6
TS _{ccdeed} (He + C ₇₀)	1.551 (<i>cc</i>), 1.730 (<i>cd</i>), 1.612 (<i>de</i>), 1.832 (<i>ee</i>)	1.666– 1.697	814.5	-953.4
TS _{ddedde} (He + C ₇₀)	1.684 (<i>dd</i>), 1.644 (<i>de</i>)	1.643– 1.677	849.4	-970.9

The B3LYP/Λ1 calculations qualitatively mimic the results obtained by PBE/3ζ though the absolute values are ~100 kJ mol⁻¹ lower in the first case. For example, the B3LYP/Λ1 activation energies increase in the series of the corresponding TSs: TS_{ccdeed}(He + C₇₀) < TS_{hex}(He + C₆₀) < TS_{ddedde}(He + C₇₀) < TS_{abccba}(He + C₇₀). The same order is observed in the case of PBE/3ζ (cf. Fig. 5 of the article).

The B3LYP/Λ1 calculations reproduces the results of scanning the triplet potential energy surface by the PBE/3ζ method (cf. Figure 1 of the article): both methods show no extremums under elongation and subsequent cleavage of the 5.6 carbon–carbon bond. The B3LYP/Λ1 plot is below.



Section B

Cartesian coordinates of the structures of endofullerenes $\text{He}_n@C_{60/70}$ ($n = 1, 2$) and transition states of their formation optimized by the PBE/3 ζ method are provided below.

He@C₆₀

6	-0.69947448	-1.24334313	3.25430490
6	0.69964378	-1.24334992	3.25431261
6	-1.42620503	0.01541033	3.25438932
6	1.42634473	0.01542195	3.25427565
6	-0.72666437	1.22708400	3.25449173
6	0.72681240	1.22709101	3.25444828
6	-1.42621707	-2.18147519	2.41504504
6	1.42633475	-2.18143013	2.41494972
6	-0.72668433	-3.08452295	1.60717132
6	0.72678918	-3.08451766	1.60713735
6	2.60222211	-0.14476311	2.41509726
6	2.60220104	-1.50249832	1.89634701
6	3.03454764	0.91269990	1.60740197
6	3.03456626	-1.75203379	0.58932445
6	3.48365691	0.65350036	0.24958453
6	3.48363859	-0.65346800	-0.24975379
6	3.03451574	1.75205967	-0.58947452
6	3.03448256	-0.91267943	-1.60755769
6	2.60208350	1.50252308	-1.89646913
6	2.60208788	0.14477990	-2.41521741
6	1.42622048	2.18148752	-2.41504813
6	1.42622221	-0.01541761	-3.25441838
6	0.69946221	1.24331522	-3.25423167
6	-2.60209304	-0.14478798	2.41522595
6	-2.60210179	-1.50253092	1.89648647
6	-3.03447176	0.91266653	1.60755231
6	-3.03449919	-1.75204697	0.58947211
6	-3.48365345	0.65346856	0.24975303
6	-3.48364985	-0.65349542	-0.24958722
6	-3.03455090	1.75202920	-0.58932676
6	-3.03455627	-0.91270112	-1.60741727
6	-2.60219645	1.50250724	-1.89634966
6	-2.60220814	0.14476109	-2.41509702
6	-1.42635617	2.18147064	-2.41497103
6	-1.42637153	-0.01543115	-3.25432985
6	-0.69963628	1.24332009	-3.25422508
6	0.72668637	3.08454298	-1.60717680
6	-0.72679550	3.08455137	-1.60714689
6	1.17586344	3.34373534	-0.24936731
6	-1.17591150	3.34373111	-0.24931394
6	-0.00000252	3.50388009	0.58982949
6	0.00003150	3.00456915	1.89680609
6	-1.17582461	2.32558995	2.41537767
6	-2.30778822	2.17144702	1.60766584
6	2.30778580	2.69019732	0.24978575
6	1.17592666	2.32562538	2.41533810
6	2.30783058	2.17146117	1.60754607
6	-2.30778621	2.69015824	0.24989477
6	-0.72681609	-1.22710210	-3.25447092
6	0.72666485	-1.22708170	-3.25446328
6	-1.17592990	-2.32562699	-2.41535077
6	1.17582566	-2.32561412	-2.41538573
6	-0.00003724	-3.00456154	-1.89679794
6	-0.00000296	-3.50390814	-0.58983375
6	-1.17587402	-3.34374852	0.24937204
6	-2.30776491	-2.69017407	-0.24978928
6	-2.30782849	-2.17144902	-1.60755228
6	1.17589607	-3.34367961	0.24930259
6	2.30781415	-2.69019045	-0.24990487
6	2.30778857	-2.17145224	-1.60766799
2	0.00000135	0.00000142	-0.00000258

He@C₆₀, TS_{hex}

6	-0.69898081	-1.29263806	3.30947185
6	0.69914895	-1.29262877	3.30943990
6	-1.42707849	-0.03427488	3.30736780
6	1.42722964	-0.03425605	3.30730271
6	-0.72571313	1.17793715	3.29636049
6	0.72584718	1.17794704	3.29632664
6	-1.42602134	-2.23116207	2.46991277
6	1.42616355	-2.23114276	2.46984673
6	-0.72696882	-3.13357997	1.66261268
6	0.72708595	-3.13356948	1.66257882
6	2.60256147	-0.19513214	2.47171569
6	2.60117674	-1.54972589	1.95156217
6	3.03440261	0.86310542	1.66273332
6	3.02653909	-1.79205012	0.63937294
6	3.47955155	0.61086595	0.30667838
6	3.47067595	-0.69078475	-0.19660898
6	3.05270839	1.72146916	-0.53256512
6	3.01885200	-0.94489998	-1.55797517
6	2.65462637	1.48282516	-1.86909294
6	2.61169696	0.10317937	-2.37700891
6	1.57668138	2.22520995	-2.42110181
6	1.44936728	-0.07300528	-3.26086044
6	0.74996436	1.15803349	-3.37573433
6	-2.60244608	-0.19516703	2.47183323
6	-2.60106826	-1.54976213	1.95168233
6	-3.03433871	0.86306334	1.66286910
6	-3.02649045	-1.79209554	0.63951457
6	-3.47954822	0.61081505	0.30683485
6	-3.47068334	-0.69083804	-0.19644804
6	-3.05275083	1.72141933	-0.53243148
6	-3.01892304	-0.94495243	-1.55783427
6	-2.65472269	1.48277175	-1.86897123
6	-2.61181784	0.10313061	-2.37688637
6	-1.57677937	2.22513795	-2.42102933
6	-1.44952846	-0.07303175	-3.26078868
6	-0.75014824	1.15802526	-3.37565541
6	0.82662308	3.19341183	-1.55491066
6	-0.82672900	3.19338202	-1.55488396
6	1.20519698	3.35389590	-0.19522597
6	-1.20524526	3.35386705	-0.19517851
6	-0.00000899	3.47466278	0.63911462
6	0.00002310	2.95214486	1.92831433
6	-1.17593491	2.27140188	2.45342278
6	-2.31114101	2.11909127	1.65606475
6	2.32999802	2.65442443	0.30205619
6	1.17601597	2.27141857	2.45337081
6	2.31118941	2.11912465	1.65596318
6	-2.33001328	2.65438581	0.30215687
6	-0.72279191	-1.28635657	-3.22317958
6	0.72265166	-1.28634405	-3.22321200
6	-1.16842651	-2.37264419	-2.36215973
6	1.16834164	-2.37262368	-2.36221266
6	-0.00002461	-3.05397630	-1.84130549
6	0.00000967	-3.55471683	-0.53361189
6	-1.17394257	-3.39206147	0.30356649
6	-2.30072260	-2.72899938	-0.19863763
6	-2.29472494	-2.20889926	-1.55450189
6	1.17399931	-3.39204311	0.30351111
6	2.30074453	-2.72896242	-0.19874536
6	2.29467392	-2.20885849	-1.55460846
2	-0.00003801	2.16504002	-2.42020130

He@C₆₀, TS_{pent}

6	-0.71066856	-1.25115669	3.26860213
6	0.68890554	-1.25249791	3.26991749
6	-1.43560326	0.00875557	3.26699853
6	1.41401207	0.00388448	3.26453280
6	-0.73307467	1.22055411	3.26012683
6	0.71971107	1.21655059	3.25260758
6	-1.43667686	-2.18815804	2.42951560
6	1.41665578	-2.19201350	2.42978191
6	-0.73700130	-3.09261131	1.62161386
6	0.71378046	-3.09621525	1.62218428
6	2.58686376	-0.16268547	2.42337322
6	2.59113169	-1.52026761	1.91235816
6	3.00512910	0.88225311	1.59592199
6	3.03177834	-1.77558303	0.60450464
6	3.48439479	0.60675102	0.26343742
6	3.51042771	-0.69805598	-0.23373538
6	3.14731598	1.73766875	-0.59215415
6	3.09213901	-0.97160482	-1.61308897
6	3.17478228	1.61454225	-1.95293474
6	2.75703597	0.06902903	-2.47791672
6	1.33903682	2.63281941	-2.75602126
6	1.47351885	-0.03381428	-3.30913162
6	0.63016450	1.34798074	-3.44198060
6	-2.61271763	-0.15299948	2.43059134
6	-2.61219287	-1.50959909	1.91125679
6	-3.04785514	0.90481639	1.62388456
6	-3.04544115	-1.75938570	0.60353065
6	-3.49822927	0.64514452	0.26437125
6	-3.49630404	-0.66402876	-0.23429859
6	-3.05563235	1.74040961	-0.57453275
6	-3.04308534	-0.92174602	-1.59000242
6	-2.62609220	1.49392390	-1.88662958
6	-2.60884881	0.13444296	-2.39624977
6	-1.48083043	2.19217587	-2.42623615
6	-1.43312454	-0.01389632	-3.23323107
6	-0.75008911	1.27316964	-3.29516935
6	0.67154485	3.16845322	-1.68545079
6	-0.77852869	3.08097434	-1.61020958
6	1.17581487	3.32355762	-0.28734395
6	-1.18874764	3.31044364	-0.24663141
6	0.00653533	3.45985913	0.56555843
6	-0.00189402	2.97817898	1.88181078
6	-1.18048322	2.31399679	2.41538811
6	-2.31991792	2.15936065	1.61999166
6	2.30576682	2.66908145	0.21261571
6	1.16388595	2.30443096	2.39562583
6	2.28109789	2.14202571	1.56643116
6	-2.32378888	2.67407012	0.26220217
6	-0.72222644	-1.21532440	-3.23294759
6	0.73863763	-1.22341013	-3.23634839
6	-1.17408609	-2.31364536	-2.39532971
6	1.17507172	-2.32410216	-2.39680362
6	-0.00414806	-2.99635100	-1.87832773
6	-0.01065641	-3.50716901	-0.57577235
6	-1.18558240	-3.35023475	0.26166791
6	-2.31567240	-2.69626594	-0.23758677
6	-2.31221747	-2.17388487	-1.59178400
6	1.16280150	-3.35401654	0.26596212
6	2.29698157	-2.70742297	-0.23284885
6	2.30797434	-2.19125366	-1.58936942
2	2.19299030	1.37669170	-3.15910387

He@C₇₀

6	-3.48314095	-0.51613462	2.20760345
6	-3.51063704	0.82232493	1.79730308
6	-3.69102287	1.15078831	0.39798787
6	-2.86835241	2.29876232	0.08481595
6	-2.16604757	2.68019938	1.28201413
6	-2.55445790	1.76811302	2.33556437
6	-2.27931309	2.46528053	-1.19911659
6	-1.10944128	3.27226138	-1.25711298
6	-0.40718105	3.65367365	-0.05988413
6	-0.85842836	3.23689365	1.22305381
6	-0.13485178	3.11903048	-2.31513286
6	1.00171196	3.73635221	-0.37755394
6	1.17770064	3.41719341	-1.77958584
6	2.29218984	2.68035650	-2.19858623
6	-2.49858785	-0.95257962	3.18149400
6	-1.58199656	-0.03262768	3.70506024
6	-1.60915148	1.34906459	3.27064681
6	-0.24781284	1.82984161	3.17951083
6	0.62919807	0.74830884	3.54442453
6	-0.18979920	-0.40127736	3.86126995
6	0.13803875	2.79519320	2.20872092
6	1.51113248	2.80336738	1.83754992
6	2.38813305	1.72183108	2.20246673
6	1.91230679	0.60714948	2.94698381
6	1.94704902	3.31732368	0.55750245
6	3.36642146	1.56699491	1.14810550
6	3.10638380	2.56226301	0.12813953
6	3.27676463	2.24392128	-1.22471070
6	-2.05174828	-2.28131795	2.80324864
6	-0.70666540	-2.63551712	2.96411657
6	0.23923352	-1.67705250	3.49809432
6	1.49979389	-1.84050643	2.80746222
6	1.33955252	-2.89037418	1.83580732
6	-0.02010709	-3.37615013	1.92555845
6	2.36456895	-0.73770058	2.56414676
6	3.25872183	-0.86698580	1.46551549
6	3.09849119	-1.91684973	0.49385461
6	2.04039121	-2.86169028	0.59838092
6	3.79545283	0.29121742	0.78493267
6	3.53612351	-1.40787446	-0.78760266
6	3.98172998	-0.04062000	-0.61280876
6	3.72360921	0.91518879	-1.60295868
6	-2.76013398	-2.66607976	1.59559464
6	-2.09433532	-3.38922834	0.59842736
6	-0.70026010	-3.74558115	0.76603639
6	-0.04060955	-3.64003897	-0.51709187
6	-1.01664197	-3.20735669	-1.48257864
6	-2.27987790	-3.04531837	-0.79649997
6	1.32341135	-3.25113344	-0.62390697
6	1.71830571	-2.66652489	-1.85902166
6	0.74222159	-2.23386908	-2.82446313
6	-0.65131527	-2.37573218	-2.57718110
6	2.85595202	-1.77731442	-1.94711006
6	1.27625620	-1.07708406	-3.50958109
6	2.59401703	-0.79434842	-2.97846317
6	3.01520300	0.53041506	-2.81059623
6	-3.64478636	-1.57513082	1.22746503
6	-3.82728481	-1.25215864	-0.12270561
6	-3.12927628	-1.99784732	-1.14995790
6	-2.74028206	-1.08178735	-2.19984126
6	-3.18327141	0.23546804	-1.82487547
6	-3.84621859	0.13399516	-0.54309797
6	-1.54663789	-1.27164853	-2.94975114
6	-0.98144627	-0.10831581	-3.54171133
6	-1.42443919	1.20893896	-3.16674948
6	-2.44290376	1.39346111	-2.19109821
6	0.42684731	-0.02962422	-3.86304021
6	-0.29007405	2.10223007	-3.25620604
6	0.86103219	1.34270215	-3.69958162
6	2.13053322	1.62135363	-3.17871666
2	0.00006130	-0.00007357	0.00002969

He@C₇₀, TS_{abcba}

6 -1.54692817 -1.73368359 -3.43212438
6 -1.54185915 -0.07549149 -3.42351580
6 -0.17744513 0.29635048 -3.30011845
6 0.66006154 -0.91222340 -3.25747442
6 -0.18481743 -2.11514115 -3.31264639
6 -2.59375930 -2.47781491 -2.63729167
6 1.80860043 -0.91981280 -2.47229362
6 0.16831943 1.40638173 -2.49394035
6 -2.58416367 0.66675645 -2.62096214
6 -0.84967268 -3.94390726 -1.75819111
6 2.17184997 -2.09049606 -1.69414806
6 2.17898083 0.24048550 -1.68204427
6 1.37206089 1.37317193 -1.68734205
6 -0.83115190 2.11290717 -1.72672915
6 -0.25910404 -4.37110233 -0.50726688
6 1.10992277 -3.93492126 -0.48298579
6 2.76979399 -1.65269673 -0.45317420
6 2.77419686 -0.21381985 -0.44570193
6 -0.23800085 2.52347589 -0.47146279
6 -2.94734812 1.67816103 -0.51565236
6 -3.83704734 0.52776355 -0.52799171
6 -3.84576559 -2.35286713 -0.54299301
6 -2.96319246 -3.50881052 -0.54260725
6 1.75370669 -3.58087492 0.73383975
6 2.61861444 -2.39614177 0.75056124
6 2.62753987 0.51800573 0.76569384
6 1.76990891 1.70812392 0.76132548
6 -0.99817455 2.60731339 0.72459310
6 -2.39797139 2.15276909 0.69931853
6 -4.13867188 -0.18403615 0.68074596
6 -4.14315939 -1.65203822 0.67308009
6 -2.41684079 -3.99942327 0.66737086
6 -1.01983237 -4.46271944 0.68787390
6 -0.29230264 -4.38322449 1.90688396
6 1.07886100 -3.94702768 1.93054938
6 -2.97919250 -3.49547553 1.87776375
6 -3.82346129 -2.33450699 1.87967408
6 -3.81453705 0.48377204 1.89422882
6 -2.96336842 1.63961911 1.90439272
6 -0.27119115 2.51071024 1.94269323
6 1.09730911 2.06596899 1.96182883
6 2.75303507 -0.22655243 1.97187197
6 2.74863935 -1.66493046 1.96439874
6 -0.91772515 -3.94880152 3.13742304
6 -2.24111867 -3.51286125 3.12193179
6 -3.60472512 -1.62825739 3.12295508
6 -3.60037684 -0.23658596 3.13014865
6 -2.22531796 1.63959408 3.14866352
6 -0.89931244 2.06727648 3.16863585
6 1.31457627 1.34387410 3.19605446
6 2.13128090 0.21432374 3.20214605
6 2.12417483 -2.11475801 3.19004726
6 1.30054200 -3.23913336 3.17220879
6 1.74958837 -0.95308983 3.97098207
6 0.08171537 1.35193491 3.95746851
6 -2.62413120 0.48187679 3.92168260
6 -2.63286090 -2.36081052 3.90694284
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6	2.10316089	2.19859358	1.83366217
6	0.89718377	2.90653378	1.83317267
6	3.04330877	0.04507304	1.83443231
6	2.74265516	-1.32063862	1.83472805
6	1.61073122	-1.81519460	2.60110722
6	0.82201816	-0.92636403	3.34266705
6	2.81605255	-2.07925072	0.59638791
6	1.72957290	-3.04336621	0.59639213
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6	-0.40670763	-3.01634592	1.83443895
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6	-1.11268866	-3.41901565	-0.52001935
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6	2.40204287	-2.44710422	-1.13177109
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6	-0.59145355	-1.08462405	3.96970224
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6	0.66027999	-0.91221225	-3.25675583
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