

Electronic Supplementary Information

Revisit of the Saito-Dresselhaus-Dresselhaus C₂ Ingestion Model: on the Mechanism of Atomic-Carbon-Participated Fullerene Growth

Wei-Wei Wang, Jing-Shuang Dang, Xiang Zhao, and Shigeru Nagase

Table S1. Energy barriers ($\Delta G^\ddagger$) of reactions at different temperatures (T)

Reactant and product	Mechanism	Rate-determining step	$\Delta G^\ddagger$ /eV			
			$T = 1000$ K	$T = 1500$ K	$T = 2000$ K	$T = 2500$ K
#6290C ₆₈ to C ₇₀	stepwise modified-SDD addition (Fig. 4)	INT-C ₆₉ C → TS-C ₆₉ C	2.19	2.33	2.49	2.66
	EK C ₂ addition and SWT reaction (Fig. 5)	hepta-C ₇₀ → TS-SW	5.52	5.40	5.30	5.21
	concerted modified-SDD addition (Fig. 6)	INT-C ₆₈ CC → TS-C ₆₈ CC	3.96	4.03	4.12	4.21
Y ₃ N@ ^{#22010} C ₇₈ to Y ₃ N@ ^{#31924} C ₈₀	stepwise modified-SDD addition (Fig 8)	INT-Y ₃ N@C ₇₉ C → TS-Y ₃ N@C ₇₉ C	2.25	2.36	2.49	2.62

Table S2. Geometric coordinates of #6290C₆₈

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.5475	-0.6561	3.4863
C	0.8928	-0.6465	3.6080
C	-0.9853	0.7051	3.5506
C	0.1621	1.5761	3.4117
C	1.3278	0.7332	3.4705
C	1.6419	-1.6734	3.0814
C	2.8733	-1.3868	2.3651
C	3.2235	-0.0621	2.1294
C	2.4376	1.0166	2.6916
C	0.1038	2.7180	2.5669
C	1.2275	2.9384	1.6452
C	2.3616	2.0872	1.7232
C	-1.2067	-1.6000	2.6646
C	-0.4313	-2.7466	2.2118
C	0.9818	-2.7821	2.4421
C	-2.2013	1.0611	3.0006
C	-2.3311	2.3620	2.4702
C	-1.2060	3.1520	2.1645
C	-2.3719	-1.1383	1.8731
C	-2.8808	0.1394	2.1095
C	1.8887	-3.3016	1.4421
C	2.9974	-2.3730	1.3205
C	-0.9174	-3.4771	1.0887
C	-0.0165	-4.1454	0.2413
C	1.3825	-3.9324	0.3125
C	-2.6560	-1.7498	0.5607
C	-2.0050	-2.9458	0.2560
C	-3.4824	0.9491	1.0414
C	-3.1985	2.2984	1.3151
C	-3.1608	-0.9089	-0.5510
C	-3.5066	0.4843	-0.3058
C	3.6221	0.3447	0.8029
C	3.6958	-0.5944	-0.2151
C	3.4214	-1.9839	0.0496
C	1.8141	-3.5108	-1.0212
C	2.7705	-2.5240	-1.1322
C	-1.4412	3.7251	0.8408
C	-0.3815	3.8969	-0.0240
C	0.9615	3.5032	0.3668
C	-2.6961	3.1767	0.3236
C	3.0641	1.6548	0.5479
C	1.6412	3.0448	-0.8045
C	2.6300	2.0274	-0.7483
C	3.1903	-0.2685	-1.5341
C	2.6839	1.0258	-1.8239
C	2.6134	-1.4491	-2.0971
C	-1.6904	-3.2964	-1.1163
C	-0.4432	-3.9557	-1.1271
C	-2.7917	-1.2623	-1.8699
C	-1.9540	-2.3937	-2.1281
C	-3.2817	1.4612	-1.3292
C	-2.7906	2.7823	-1.0049
C	-2.4591	-0.2534	-2.8499
C	-2.6792	1.0778	-2.5798
C	0.6396	-3.4776	-1.8901
C	1.4812	-1.3818	-2.9562
C	0.4364	-2.4078	-2.8282
C	-0.9086	-2.0053	-3.0508
C	-1.2399	-0.6827	-3.5138
C	-1.7250	3.1031	-1.9358
C	-0.5348	3.6418	-1.4466
C	-1.6823	2.0711	-2.9419
C	-0.2407	0.2456	-3.7561
C	-0.4661	1.6462	-3.4641
C	0.7260	3.1348	-1.9253
C	0.7647	2.1753	-2.9263
C	1.7289	1.0989	-2.8678
C	1.1237	-0.0847	-3.4106

Table S3. Geometric coordinates of C₇₀

Atom	X (Å)	Y (Å)	Z (Å)
C	2.8370	2.3177	1.9487
C	3.5543	1.5788	1.0101
C	3.3868	1.8386	-0.4023
C	3.4449	0.5791	-1.1120
C	2.6938	0.3592	-2.2944
C	2.3866	-0.9909	-2.6008
C	1.2436	-1.3396	-3.4167
C	0.7281	-2.6132	-2.9657
C	-0.6455	-2.8459	-2.9483
C	-1.2480	-3.5161	-1.8133
C	-2.5319	-2.8948	-1.5557
C	-2.9591	-2.7082	-0.2427
C	-3.5841	-1.4643	0.1484
C	-3.1519	-1.1336	1.4888
C	-2.9954	0.2124	1.9063
C	-2.0938	0.4360	2.9775
C	-1.4409	1.7139	3.1620
C	-0.1322	1.4838	3.7322
C	0.9506	2.2692	3.3420
C	2.2344	1.6474	3.0842
C	1.9255	3.3539	1.5048
C	0.7596	3.3239	2.3657
C	-0.5055	3.5449	1.8248

C	-1.6234	2.7217	2.2290
C	-2.4656	2.4900	1.0757
C	-3.1887	1.2807	0.9174
C	-3.5245	0.9207	-0.4124
C	-3.7666	-0.4563	-0.7846
C	-3.3323	-0.6470	-2.1504
C	-2.7229	-1.8405	-2.5319
C	-1.5572	-1.8104	-3.3930
C	-1.0540	-0.5881	-3.8339
C	0.3721	-0.3494	-3.8405
C	0.6105	1.0274	-3.4656
C	1.7705	1.4085	-2.7443
C	1.6689	2.5964	-1.9768
C	2.5154	2.8285	-0.8266
C	1.7730	3.6035	0.1422
C	0.4570	3.8246	-0.4138
C	-0.6573	3.7964	0.4090
C	-1.8703	3.1522	-0.0458
C	-1.9820	2.6232	-1.3567
C	-2.9292	1.5828	-1.5340
C	-2.8006	0.6184	-2.6048
C	-1.6864	0.6474	-3.4279
C	-0.6580	1.6419	-3.2120
C	-0.8014	2.6542	-2.2292

C	0.4006	3.2107	-1.7227
C	3.6925	0.1478	1.1626
C	3.6337	-0.4627	-0.1477
C	3.0765	-1.7526	-0.3398
C	2.5754	-2.0327	-1.6365
C	1.5500	-3.0305	-1.8515
C	0.9740	-3.6710	-0.7662
C	-0.4496	-3.9234	-0.7464
C	-0.8952	-3.7194	0.6140
C	-2.1224	-3.1251	0.8603
C	-2.2518	-2.1573	1.9278
C	-1.1696	-1.8623	2.7953
C	-1.1930	-0.5874	3.4159
C	0.0208	0.0530	3.8737
C	1.2478	-0.5412	3.6274
C	2.3771	0.2688	3.2294
C	3.1168	-0.4929	2.2477
C	2.4596	-1.7685	2.0636
C	2.4657	-2.4313	0.8102
C	1.4013	-3.3380	0.5753
C	0.2495	-3.3686	1.4261
C	0.1309	-2.4928	2.5351
C	1.3077	-1.7983	2.9138

Table S4. Geometric coordinates of INT1-C₆₈C

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.8584	2.4031	-2.3942
C	-1.4798	3.1594	-1.3199
C	0.5299	2.7510	-2.3652
C	0.8343	3.4566	-1.1382
C	-0.4229	3.7179	-0.4976
C	-2.6426	2.7247	-0.7341
C	-2.8108	2.7456	0.7063
C	-1.7478	3.1553	1.4979
C	-0.5333	3.6557	0.8839
C	2.0059	3.1479	-0.3978
C	1.8574	2.9461	1.0496
C	0.5976	3.1972	1.6562
C	-1.3287	1.1268	-2.8130
C	-2.7111	0.8293	-2.3332
C	-3.2803	1.5638	-1.2646
C	1.4615	1.9127	-2.9321
C	2.7588	1.8983	-2.3768
C	3.0236	2.4107	-1.0937
C	-0.2431	0.0957	-3.2135
C	1.0799	0.5589	-3.2873
C	-3.9739	0.9067	-0.1704
C	-3.5916	1.5810	1.0543
C	-3.2310	-0.5009	-2.4884

C	-3.7347	-1.1853	-1.3674
C	-4.0938	-0.4772	-0.1899
C	-0.3351	-1.4017	-3.0179
C	-1.6132	-1.9795	-2.9290
C	2.2540	-0.2829	-2.9562
C	3.2727	0.5523	-2.4704
C	0.7694	-2.1466	-2.4259
C	2.0974	-1.5777	-2.3917
C	-1.3576	2.3575	2.6362
C	-2.0687	1.2076	2.9484
C	-3.2258	0.8238	2.1703
C	-3.6656	-1.2641	0.9493
C	-3.2241	-0.6220	2.0923
C	3.8464	1.4175	-0.4048
C	3.6679	1.2100	0.9470
C	2.6718	1.9684	1.6867
C	3.9958	0.2585	-1.2858
C	0.0879	2.3655	2.7126
C	2.1472	1.1204	2.7101
C	0.8045	1.2303	3.1630
C	-1.3569	0.0085	3.3367
C	0.0563	0.0044	3.4757
C	-2.0594	-1.1157	2.7991
C	-1.9289	-2.8007	-1.7581

C	-3.0516	-2.4081	-0.9818
C	0.4754	-3.2099	-1.5441
C	-0.8652	-3.4019	-1.0890
C	3.0141	-1.9817	-1.3739
C	3.9061	-1.0283	-0.7641
C	1.3570	-3.5107	-0.4403
C	2.5937	-2.9071	-0.3480
C	-2.9808	-2.4392	0.4471
C	-1.3750	-2.2811	2.3646
C	-1.8312	-2.9502	1.1346
C	-0.8508	-3.5839	0.3380
C	0.5281	-3.6753	0.7398
C	3.8586	-1.2360	0.6724
C	3.7296	-0.1300	1.5104
C	3.0774	-2.4240	0.9301
C	0.9440	-3.1247	1.9427
C	2.2389	-2.4897	2.0400
C	2.7986	-0.1715	2.6107
C	2.0820	-1.3267	2.8841
C	0.6961	-1.2460	3.2914
C	-0.0041	-2.3667	2.7290
C	-2.6420	-1.2220	-3.5522

Table S5. Geometric coordinates of TS-C₆₈C

Atom	X (Å)	Y (Å)	Z (Å)
C	1.3480	-2.2522	-2.5023
C	2.0526	-2.9175	-1.4232
C	0.0122	-2.7384	-2.5002
C	-0.2097	-3.5275	-1.3056
C	1.0639	-3.6346	-0.6415
C	3.1208	-2.3068	-0.8038
C	3.2436	-2.3205	0.6410
C	2.2457	-2.9261	1.3964
C	1.1377	-3.5967	0.7434
C	-1.4219	-3.4156	-0.5784
C	-1.3373	-3.2687	0.8794
C	-0.0647	-3.3487	1.5064
C	1.6281	-0.9242	-2.8824
C	2.8731	-0.3881	-2.3383
C	3.5582	-1.0323	-1.2928
C	-0.9908	-1.9405	-3.0154
C	-2.2779	-2.1394	-2.4940
C	-2.5106	-2.7834	-1.2652
C	0.5207	-0.0032	-3.3441
C	-0.7863	-0.5190	-3.3388
C	4.0468	-0.2648	-0.1643
C	3.7908	-1.0419	1.0365
C	2.9358	1.0369	-2.4027

C	3.3543	1.7846	-1.2892
C	3.8992	1.1194	-0.1449
C	-0.0939	2.0620	-3.1767
C	1.1579	2.5544	-2.8507
C	-2.1243	0.1306	-2.9615
C	-2.9845	-0.8873	-2.5330
C	-1.2041	2.3286	-2.3476
C	-2.3149	1.4163	-2.3418
C	1.7118	-2.2453	2.5524
C	2.2182	-1.0083	2.9238
C	3.2902	-0.4024	2.1700
C	3.3609	1.7758	1.0293
C	3.0421	1.0256	2.1469
C	-3.5019	-1.9821	-0.5555
C	-3.4040	-1.8411	0.8149
C	-2.3102	-2.4671	1.5402
C	-3.8083	-0.8088	-1.3705
C	0.2875	-2.4952	2.6061
C	-1.9481	-1.6028	2.6196
C	-0.6113	-1.5156	3.0931
C	1.3134	0.0380	3.3527
C	-0.0793	-0.1996	3.4753
C	1.8202	1.2891	2.8738
C	1.3984	3.2748	-1.6103

C	2.5291	2.8899	-0.8450
C	-1.0574	3.3022	-1.3409
C	0.2583	3.6670	-0.8833
C	-3.2863	1.5624	-1.3109
C	-3.9856	0.4261	-0.7711
C	-1.9649	3.3383	-0.2291
C	-3.0538	2.4859	-0.2164
C	2.4820	2.8407	0.5881
C	0.9531	2.3470	2.4971
C	1.2887	3.1460	1.3069
C	0.2182	3.6917	0.5494
C	-1.1604	3.5326	0.9601
C	-4.0027	0.5470	0.6742
C	-3.6995	-0.5689	1.4503
C	-3.4494	1.8361	1.0184
C	-1.4710	2.8254	2.1080
C	-2.6424	1.9756	2.1455
C	-2.8029	-0.4339	2.5735
C	-2.2972	0.8083	2.9238
C	-0.9176	0.9370	3.3447
C	-0.4117	2.1853	2.8561
C	2.0251	1.5680	-3.3257

Table S6. Geometric coordinates of INT2-C₆₈C

Atom	X (Å)	Y (Å)	Z (Å)
C	2.2102	-1.7229	-2.5629
C	3.0584	-2.0881	-1.4476
C	1.0465	-2.5397	-2.5402
C	1.0774	-3.3620	-1.3549
C	2.3208	-3.0675	-0.6727
C	3.8275	-1.1222	-0.8146
C	3.8919	-1.0766	0.6346
C	3.1497	-1.9909	1.3771
C	2.3479	-3.0003	0.7121
C	-0.1126	-3.6569	-0.6388
C	-0.0966	-3.5265	0.8226
C	1.1228	-3.1792	1.4624
C	2.0664	-0.4023	-2.9554
C	2.9358	0.5722	-2.3498
C	3.7974	0.2365	-1.3017
C	-0.1599	-2.0203	-3.0160
C	-1.3092	-2.6312	-2.5141
C	-1.3359	-3.3892	-1.3262
C	0.7587	0.2296	-3.2869
C	-0.4154	-0.5802	-3.2643
C	3.9115	1.1319	-0.1645
C	3.9376	0.3160	1.0340
C	2.2483	1.8249	-2.3454

C	2.4309	2.7299	-1.3057
C	3.2340	2.3478	-0.1664
C	-1.2648	2.3197	-3.3779
C	-0.0143	2.6373	-2.8136
C	-1.9456	-0.4135	-2.8999
C	-2.3875	-1.6881	-2.5247
C	-2.2315	2.0272	-2.4020
C	-2.7448	0.6828	-2.3421
C	2.4020	-1.5443	2.5293
C	2.4419	-0.2126	2.9124
C	3.2347	0.7353	2.1634
C	2.5154	2.7841	1.0142
C	2.5010	1.9822	2.1440
C	-2.5495	-3.0040	-0.6208
C	-2.5264	-2.8919	0.7563
C	-1.2898	-3.1225	1.4837
C	-3.2273	-1.9738	-1.4037
C	1.1525	-2.2728	2.5724
C	-1.2547	-2.2103	2.5861
C	-0.0318	-1.6736	3.0688
C	1.2315	0.4476	3.3509
C	0.0089	-0.2608	3.4718
C	1.2677	1.8004	2.8795
C	0.0812	3.4385	-1.5774

C	1.2823	3.4545	-0.8396
C	-2.3014	2.8667	-1.2754
C	-1.1154	3.5643	-0.8361
C	-3.6563	0.4036	-1.2803
C	-3.8598	-0.9224	-0.7721
C	-3.0826	2.5079	-0.1379
C	-3.7902	1.3167	-0.1552
C	1.3029	3.4555	0.5922
C	0.0802	2.4909	2.5213
C	0.0973	3.3579	1.3319
C	-1.1115	3.5391	0.6001
C	-2.3423	2.9161	1.0378
C	-3.9307	-0.8660	0.6734
C	-3.2538	-1.8243	1.4214
C	-3.8887	0.5259	1.0566
C	-2.3646	2.1161	2.1661
C	-3.1670	0.9117	2.1867
C	-2.4633	-1.4129	2.5567
C	-2.4238	-0.0786	2.9330
C	-1.1743	0.5132	3.3616
C	-1.1380	1.8655	2.8916
C	0.9886	1.6790	-3.0194

Table S7. Geometric coordinates of INT-C₆₉C

Atom	X (Å)	Y (Å)	Z (Å)
C	2.1423	-0.3826	-3.0938
C	3.1371	-1.0047	-2.2447
C	1.0905	-1.3111	-3.3160
C	1.3383	-2.5004	-2.5342
C	2.6028	-2.2972	-1.8592
C	3.8542	-0.2395	-1.3373
C	4.0628	-0.7203	0.0160
C	3.5118	-1.9402	0.3973
C	2.7667	-2.7409	-0.5555
C	0.2709	-3.2046	-1.9206
C	0.4233	-3.6190	-0.5209
C	1.6551	-3.3577	0.1361
C	1.8072	0.9569	-2.9541
C	2.6218	1.7560	-2.0712
C	3.6193	1.1839	-1.2736
C	-0.2086	-0.8335	-3.4848
C	-1.2241	-1.7413	-3.1959
C	-1.0410	-2.8780	-2.3872
C	0.4075	1.4630	-2.9541
C	-0.6513	0.5437	-3.1655
C	3.7445	1.6046	0.1084
C	3.9908	0.4194	0.9080
C	1.8095	2.8107	-1.5575

C	1.9820	3.2802	-0.2595
C	2.9375	2.6243	0.6043
C	-1.8870	3.2450	-2.1157
C	-0.5361	3.3938	-1.5261
C	-2.1400	0.3569	-2.6857
C	-2.3938	-1.0175	-2.7860
C	-2.7306	2.3928	-1.2773
C	-2.9925	1.0528	-1.7034
C	2.8428	-2.0611	1.6717
C	2.7711	-0.9725	2.5272
C	3.3673	0.2888	2.1482
C	2.3024	2.4866	1.8986
C	2.4993	1.3355	2.6429
C	-2.2099	-2.9574	-1.5235
C	-2.0573	-3.3597	-0.2121
C	-0.7327	-3.6619	0.3073
C	-3.0762	-1.8172	-1.8197
C	1.6964	-2.9280	1.5037
C	-0.6877	-3.2234	1.6678
C	0.5096	-2.7281	2.2505
C	1.5458	-0.7008	3.2463
C	0.4316	-1.5724	3.1551
C	1.3781	0.7217	3.3193
C	-0.4471	3.7091	-0.1096

C	0.8164	3.6196	0.5122
C	-2.7491	2.7330	0.0710
C	-1.5821	3.3858	0.6839
C	-3.7602	0.2570	-0.7816
C	-3.7563	-1.1767	-0.8053
C	-3.3085	1.8431	1.0295
C	-3.8818	0.6573	0.6049
C	0.9879	3.0902	1.8315
C	0.0889	1.3164	3.3078
C	-0.1159	2.5535	2.5349
C	-1.4086	2.8153	1.9846
C	-2.5013	1.8950	2.2251
C	-3.6866	-1.6720	0.5547
C	-2.8274	-2.7265	0.8459
C	-3.7631	-0.5295	1.4328
C	-2.3181	0.7478	2.9714
C	-2.9729	-0.4842	2.5798
C	-1.9763	-2.6540	2.0081
C	-2.0494	-1.5599	2.8584
C	-0.8372	-0.9907	3.4089
C	-1.0036	0.4291	3.4844
C	0.4953	2.7286	-2.1460
C	-1.9945	3.8665	-3.2613

Table S8. Geometric coordinates of TS-C₆₉C

Atom	X (Å)	Y (Å)	Z (Å)
C	2.2668	-1.0286	-2.8690
C	3.1473	-1.6042	-1.8783
C	1.1189	-1.8638	-2.9953
C	1.1950	-2.9202	-2.0395
C	2.4487	-2.7553	-1.3318
C	3.8881	-0.7684	-1.0545
C	3.9738	-1.0420	0.3681
C	3.2810	-2.1318	0.8953
C	2.4967	-2.9913	0.0318
C	0.0113	-3.4163	-1.3923
C	0.0674	-3.6273	0.0546
C	1.2923	-3.3865	0.7391
C	2.1064	0.3444	-2.9765
C	2.9533	1.2044	-2.1881
C	3.8121	0.6647	-1.2298
C	-0.1295	-1.2670	-3.2386
C	-1.2848	-2.0268	-2.9843
C	-1.2298	-3.0460	-1.9723
C	0.7762	0.9880	-3.0840
C	-0.3740	0.1239	-3.0553
C	3.8930	1.2845	0.0816
C	3.9727	0.2252	1.0657
C	2.2185	2.4165	-1.9197

C	2.3273	3.0362	-0.6722
C	3.1523	2.4353	0.3487
C	-1.3802	2.6312	-2.6847
C	-0.1626	3.0958	-2.1225
C	-1.9803	0.2803	-2.9078
C	-2.3890	-1.1783	-2.8295
C	-2.4044	2.3708	-1.7407
C	-2.8386	1.0422	-1.9222
C	2.5438	-1.9887	2.1272
C	2.5393	-0.7775	2.7956
C	3.2759	0.3482	2.2717
C	2.4305	2.5530	1.6006
C	2.4839	1.5254	2.5308
C	-2.4262	-2.8894	-1.1905
C	-2.3737	-3.1073	0.1838
C	-1.1205	-3.4512	0.8141
C	-3.1526	-1.7395	-1.7206
C	1.3178	-2.7590	2.0185
C	-1.0859	-2.8151	2.1062
C	0.1231	-2.3469	2.6700
C	1.3117	-0.2901	3.3997
C	0.1238	-1.0624	3.3841
C	1.2792	1.1286	3.2334
C	-0.1025	3.6057	-0.7533

C	1.1301	3.5483	-0.0500
C	-2.4791	2.9729	-0.4855
C	-1.2789	3.5471	0.0457
C	-3.7228	0.4964	-1.0006
C	-3.8102	-0.9228	-0.8229
C	-3.2003	2.3215	0.5724
C	-3.8564	1.1278	0.3065
C	1.1849	3.2344	1.3474
C	0.0559	1.8281	3.0600
C	0.0051	2.9254	2.0851
C	-1.2279	3.2146	1.4522
C	-2.4257	2.4748	1.7792
C	-3.8565	-1.1984	0.5989
C	-3.1267	-2.2712	1.0986
C	-3.8725	0.0698	1.2943
C	-2.3857	1.4370	2.7048
C	-3.1340	0.2259	2.4707
C	-2.3264	-2.0919	2.2863
C	-2.3269	-0.8763	2.9544
C	-1.0926	-0.3401	3.4774
C	-1.1261	1.0860	3.3179
C	0.9519	2.3428	-2.5715
C	-1.4726	1.8248	-3.8883

Table S9. Geometric coordinates of INT-C₆₈C₂

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.5554	-0.6918	3.5377
C	0.8858	-0.6751	3.6461
C	-1.0102	0.6675	3.5555
C	0.1272	1.5267	3.4016
C	1.3065	0.7029	3.4858
C	1.6373	-1.7026	3.1170
C	2.8613	-1.4146	2.3921
C	3.2072	-0.0882	2.1525
C	2.4160	0.9884	2.7090
C	0.0455	2.6462	2.5446
C	1.1882	2.8936	1.6471
C	2.3324	2.0554	1.7362
C	-1.1970	-1.6450	2.7231
C	-0.4306	-2.7737	2.2523
C	0.9790	-2.8151	2.4782
C	-2.2775	0.9863	3.0706
C	-2.4350	2.2549	2.4317
C	-1.2723	3.0331	2.1315
C	-2.4389	-1.2456	2.0434
C	-3.0657	-0.1138	2.5476
C	1.8730	-3.3325	1.4705
C	2.9819	-2.4034	1.3454
C	-0.9492	-3.4755	1.1311

C	-0.0591	-4.1418	0.2765
C	1.3466	-3.9519	0.3424
C	-2.7427	-1.7398	0.6490
C	-2.0470	-2.9072	0.3111
C	-3.9909	1.1569	0.8734
C	-3.3269	2.3258	1.2636
C	-3.2497	-0.8565	-0.5020
C	-3.6837	0.5653	-0.3888
C	3.6033	0.3174	0.8234
C	3.6749	-0.6230	-0.1932
C	3.3964	-2.0131	0.0730
C	1.7752	-3.5313	-0.9923
C	2.7396	-2.5518	-1.1071
C	-1.4607	3.6451	0.8280
C	-0.3936	3.8588	-0.0215
C	0.9432	3.4687	0.3733
C	-2.7101	3.1537	0.2919
C	3.0457	1.6281	0.5657
C	1.6370	3.0228	-0.7964
C	2.6209	2.0019	-0.7341
C	3.1729	-0.2981	-1.5138
C	2.6753	0.9994	-1.8087
C	2.5893	-1.4761	-2.0741
C	-1.7240	-3.2555	-1.0607

C	-0.4896	-3.9382	-1.0866
C	-2.8118	-1.2136	-1.8065
C	-1.9781	-2.3502	-2.0635
C	-3.3168	1.5023	-1.3965
C	-2.8106	2.8097	-1.0489
C	-2.4711	-0.2360	-2.8274
C	-2.6784	1.1018	-2.6096
C	0.5965	-3.4838	-1.8565
C	1.4584	-1.4017	-2.9348
C	0.4030	-2.4149	-2.7955
C	-0.9372	-1.9948	-3.0045
C	-1.2556	-0.6805	-3.4849
C	-1.7230	3.1175	-1.9608
C	-0.5328	3.6333	-1.4495
C	-1.6731	2.0843	-2.9675
C	-0.2482	0.2361	-3.7466
C	-0.4575	1.6437	-3.4733
C	0.7319	3.1226	-1.9230
C	0.7730	2.1637	-2.9258
C	1.7273	1.0778	-2.8582
C	1.1128	-0.1039	-3.3967
C	-5.4363	-0.3187	2.4521
C	-4.3785	0.2548	1.9581

Table S10. Geometric coordinates of TS-C₆₈C₂

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.7627	-3.4045	-0.9872
C	-1.7403	-2.8397	-1.8677
C	0.5351	-3.2762	-1.6190
C	0.3933	-2.4377	-2.7622
C	-1.0181	-2.1855	-2.9428
C	-2.9002	-2.2751	-1.3527
C	-3.4181	-1.0428	-1.9120
C	-2.6787	-0.3796	-2.8877
C	-1.4540	-0.9583	-3.4023
C	1.3784	-1.4524	-3.0460
C	0.9056	-0.1210	-3.4652
C	-0.4901	0.1012	-3.6147
C	-0.9060	-3.2018	0.4095
C	-2.1271	-2.6833	0.9631
C	-3.1522	-2.2663	0.0658
C	1.7171	-3.3139	-0.8614
C	2.8097	-2.5014	-1.2770
C	2.6182	-1.5601	-2.3468
C	0.3163	-3.0035	1.1193
C	1.5340	-3.4377	0.5577
C	-3.9692	-1.1080	0.3658
C	-4.0405	-0.3043	-0.8339
C	-2.0384	-2.0866	2.2619

C	-3.0061	-1.1092	2.5983
C	-3.8346	-0.5043	1.6085
C	0.5146	-2.1491	2.3787
C	-0.7645	-1.7640	2.9346
C	3.3385	-2.0591	1.0974
C	3.6382	-1.8646	-0.2586
C	1.7093	-0.9666	2.6202
C	2.9886	-0.9162	1.8850
C	-2.4594	1.0414	-2.7744
C	-3.0204	1.7462	-1.7206
C	-3.8585	1.0777	-0.7502
C	-3.6280	0.9419	1.6972
C	-3.6046	1.6969	0.5334
C	3.3873	-0.3700	-2.0374
C	2.9388	0.8827	-2.4206
C	1.6784	1.0166	-3.1175
C	3.9836	-0.5530	-0.7340
C	-1.1057	1.3292	-3.2080
C	1.0595	2.2340	-2.6838
C	-0.3515	2.3668	-2.6056
C	-2.2435	2.7578	-1.0371
C	-0.9384	3.0979	-1.4729
C	-2.5913	2.7173	0.3541
C	-1.0057	-0.4735	3.5519

C	-2.3425	-0.0733	3.3191
C	1.3020	0.2432	3.2082
C	-0.0567	0.5352	3.5868
C	3.5456	0.3224	1.5068
C	4.0397	0.5122	0.1547
C	1.9106	1.5034	2.8289
C	2.9765	1.5445	1.9517
C	-2.6569	1.1947	2.7437
C	-1.6252	2.9870	1.3638
C	-1.6407	2.1775	2.5881
C	-0.3785	1.8706	3.1890
C	0.8419	2.4748	2.7172
C	3.6375	1.8419	-0.2616
C	3.0906	2.0182	-1.5329
C	3.0234	2.5068	0.8688
C	0.8350	3.3478	1.6422
C	1.9355	3.3495	0.6936
C	1.9261	2.8557	-1.7058
C	1.3679	3.5207	-0.6222
C	-0.0686	3.6210	-0.4815
C	-0.3981	3.5461	0.9115
C	1.8800	-3.1870	2.7914
C	2.5185	-3.1515	1.5356

Table S11. Geometric coordinates of hepta-C₇₀

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.4801	-0.7212	3.6990
C	0.9636	-0.6706	3.7057
C	-0.9625	0.6280	3.5972
C	0.1685	1.5018	3.3922
C	1.3599	0.7046	3.4867
C	1.7066	-1.7056	3.1705
C	2.8939	-1.4146	2.3937
C	3.2428	-0.0883	2.1344
C	2.4589	0.9873	2.6876
C	0.0788	2.6068	2.5147
C	1.2190	2.8768	1.6242
C	2.3664	2.0475	1.7102
C	-1.1602	-1.7920	3.0640
C	-0.3831	-2.8803	2.4801
C	1.0352	-2.8526	2.5806
C	-2.2271	0.9223	3.0389
C	-2.3706	2.1654	2.3479
C	-1.2319	2.9803	2.0834
C	-2.4377	-1.4970	2.5057
C	-3.0005	-0.1983	2.5898
C	1.8769	-3.3328	1.5118
C	2.9802	-2.4044	1.3467
C	-0.9402	-3.5423	1.3304

C	-0.0936	-4.1072	0.3797
C	1.3086	-3.9391	0.3906
C	-2.8938	-2.0760	1.2277
C	-2.1070	-3.0142	0.6112
C	-4.0016	1.1931	0.7687
C	-3.2916	2.3007	1.2207
C	-3.7946	-0.5939	-0.7560
C	-4.0280	0.8574	-0.6398
C	3.6175	0.3053	0.7949
C	3.6628	-0.6393	-0.2188
C	3.3665	-2.0233	0.0618
C	1.6864	-3.5074	-0.9526
C	2.6701	-2.5519	-1.0991
C	-1.4361	3.6416	0.8105
C	-0.3656	3.8720	-0.0343
C	0.9687	3.4640	0.3562
C	-2.7053	3.2064	0.2686
C	3.0715	1.6202	0.5340
C	1.6590	3.0276	-0.8170
C	2.6372	1.9972	-0.7598
C	3.1398	-0.3119	-1.5313
C	2.6621	0.9920	-1.8298
C	2.5171	-1.4818	-2.0668
C	-1.8377	-3.1366	-0.8508

C	-0.6055	-3.8196	-0.9480
C	-3.0546	-1.0660	-1.8501
C	-2.1248	-2.1969	-1.8642
C	-3.4942	1.7532	-1.5548
C	-2.8332	2.9626	-1.1002
C	-2.5841	-0.1099	-2.8431
C	-2.7767	1.2597	-2.7032
C	0.4711	-3.4061	-1.7544
C	1.3584	-1.3835	-2.8863
C	0.2707	-2.3430	-2.6749
C	-1.0680	-1.8867	-2.8210
C	-1.3481	-0.6028	-3.3948
C	-1.7118	3.2124	-1.9842
C	-0.5061	3.6786	-1.4603
C	-1.6944	2.1779	-2.9981
C	-0.3150	0.2743	-3.7019
C	-0.4832	1.6920	-3.4789
C	0.7506	3.1447	-1.9373
C	0.7626	2.1841	-2.9363
C	1.6968	1.0813	-2.8641
C	1.0412	-0.0900	-3.3663
C	-3.7805	-1.1134	0.5975
C	-3.8944	-0.0322	1.4835

Table S12. Geometric coordinates of TS-SW

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.4169	-0.7433	3.7533
C	1.0247	-0.6641	3.7488
C	-0.9303	0.5911	3.5645
C	0.1830	1.4857	3.3780
C	1.3904	0.7118	3.4914
C	1.7865	-1.6952	3.2221
C	2.9460	-1.4003	2.4069
C	3.2743	-0.0735	2.1311
C	2.4835	1.0000	2.6865
C	0.0916	2.5895	2.4990
C	1.2326	2.8806	1.6189
C	2.3831	2.0568	1.7045
C	-1.0820	-1.8539	3.2147
C	-0.2884	-2.9555	2.6587
C	1.1238	-2.8574	2.6752
C	-2.1749	0.8280	2.9424
C	-2.3291	2.0824	2.2866
C	-1.2148	2.9419	2.0608
C	-2.3698	-1.6218	2.6051
C	-2.9360	-0.3238	2.4684
C	1.9052	-3.3226	1.5519
C	3.0025	-2.3941	1.3564
C	-0.8905	-3.6803	1.5977

C	-0.1632	-4.0509	0.4950
C	1.2609	-3.8739	0.4476
C	-2.7173	-2.5094	1.5514
C	-2.5279	-2.9294	0.3902
C	-3.9388	1.1481	0.7028
C	-3.2512	2.2451	1.1738
C	-3.9059	-0.5511	-0.8906
C	-4.0414	0.9045	-0.7140
C	3.6342	0.3176	0.7872
C	3.6665	-0.6290	-0.2249
C	3.3599	-2.0117	0.0640
C	1.6069	-3.4387	-0.8899
C	2.6273	-2.5264	-1.0744
C	-1.4257	3.6328	0.8031
C	-0.3535	3.8872	-0.0351
C	0.9800	3.4749	0.3549
C	-2.6890	3.2024	0.2503
C	3.0877	1.6340	0.5282
C	1.6720	3.0434	-0.8197
C	2.6481	2.0107	-0.7633
C	3.1338	-0.3009	-1.5315
C	2.6648	1.0046	-1.8330
C	2.4818	-1.4647	-2.0480
C	-1.9635	-3.0730	-0.9024

C	-0.6938	-3.7117	-0.8279
C	-3.1430	-1.0197	-1.9732
C	-2.2092	-2.1508	-1.9572
C	-3.4971	1.8117	-1.6043
C	-2.8197	3.0001	-1.1231
C	-2.6127	-0.0495	-2.9270
C	-2.7811	1.3224	-2.7610
C	0.3821	-3.3191	-1.6603
C	1.3213	-1.3577	-2.8597
C	0.2114	-2.2924	-2.6264
C	-1.1144	-1.8384	-2.8477
C	-1.3663	-0.5515	-3.4399
C	-1.6951	3.2542	-1.9988
C	-0.4895	3.7052	-1.4626
C	-1.6827	2.2289	-3.0263
C	-0.3172	0.3130	-3.7192
C	-0.4712	1.7309	-3.4951
C	0.7676	3.1681	-1.9408
C	0.7763	2.2101	-2.9421
C	1.6998	1.0993	-2.8669
C	1.0292	-0.0671	-3.3622
C	-3.9636	-1.1678	0.4086
C	-3.8255	-0.1460	1.3521

Table S13. Geometric coordinates of INT-C₆₈CC

Atom	X (Å)	Y (Å)	Z (Å)
C	0.5231	-2.8681	-2.0586
C	1.2207	-3.4569	-0.9303
C	-0.8739	-3.0402	-1.8062
C	-1.0669	-3.4931	-0.4561
C	0.2344	-3.7628	0.0864
C	2.4702	-3.0124	-0.5603
C	2.7985	-2.7788	0.8289
C	1.8147	-2.9651	1.7928
C	0.5128	-3.4715	1.4149
C	-2.1163	-2.9537	0.3181
C	-1.7976	-2.5511	1.6960
C	-0.4931	-2.7964	2.2029
C	1.0238	-1.7264	-2.7383
C	2.4469	-1.4419	-2.4750
C	3.1035	-2.0081	-1.3604
C	-1.8182	-2.2800	-2.4847
C	-3.0218	-1.9687	-1.7918
C	-3.1440	-2.2588	-0.3976
C	0.0028	-0.7958	-3.3559
C	-1.3064	-1.3069	-3.4468
C	3.9405	-1.2053	-0.4929
C	3.6711	-1.6229	0.8694
C	2.9589	-0.1847	-2.9359

C	3.6236	0.6551	-2.0269
C	4.1033	0.1461	-0.7883
C	0.0045	0.7835	-3.3578
C	1.3138	1.2943	-3.4487
C	-2.9520	0.1734	-2.9389
C	-3.6174	-0.6642	-2.0284
C	-1.0171	1.7156	-2.7433
C	-2.4404	1.4317	-2.4805
C	1.6038	-1.9508	2.8015
C	2.4033	-0.8180	2.8186
C	3.4736	-0.6564	1.8570
C	3.8482	1.1485	0.2267
C	3.5255	0.7499	1.5126
C	-3.8441	-1.1522	0.2261
C	-3.5225	-0.7506	1.5113
C	-2.4796	-1.4365	2.2491
C	-4.0983	-0.1523	-0.7916
C	0.1799	-1.8418	3.0402
C	-1.8009	-0.4739	3.0594
C	-0.4191	-0.6004	3.3638
C	1.8026	0.4769	3.0598
C	0.4205	0.6042	3.3627
C	2.4820	1.4375	2.2478
C	1.8247	2.2697	-2.4885

C	3.0278	1.9601	-1.7938
C	-0.5169	2.8589	-2.0659
C	0.8798	3.0316	-1.8127
C	-3.0979	2.0005	-1.3679
C	-3.9357	1.1998	-0.4992
C	-1.2156	3.4504	-0.9396
C	-2.4654	3.0068	-0.5697
C	3.1487	2.2535	-0.4003
C	1.8005	2.5509	1.6915
C	2.1204	2.9501	0.3129
C	1.0716	3.4876	-0.4635
C	-0.2301	3.7587	0.0772
C	-3.6675	1.6207	0.8623
C	-3.4709	0.6565	1.8523
C	-2.7949	2.7765	0.8198
C	-0.5097	3.4705	1.4061
C	-1.8119	2.9650	1.7841
C	-2.4015	0.8204	2.8145
C	-1.6019	1.9532	2.7954
C	-0.1782	1.8447	3.0356
C	0.4955	2.7973	2.1966
C	2.2439	0.3778	-4.0173
C	-2.2361	-0.3917	-4.0184

Table S14. Geometric coordinates of TS-C₆₈CC

Atom	X (Å)	Y (Å)	Z (Å)
C	1.3839	-2.2166	-2.4909
C	2.0789	-2.8892	-1.4141
C	0.0350	-2.6838	-2.4897
C	-0.1883	-3.4650	-1.3056
C	1.0813	-3.5997	-0.6408
C	3.1494	-2.2873	-0.7819
C	3.2645	-2.3105	0.6578
C	2.2587	-2.9165	1.4054
C	1.1524	-3.5751	0.7445
C	-1.4026	-3.3283	-0.5982
C	-1.3245	-3.2258	0.8672
C	-0.0550	-3.3234	1.4996
C	1.6870	-0.8773	-2.8248
C	2.9415	-0.3581	-2.3112
C	3.6061	-1.0108	-1.2558
C	-0.9699	-1.9474	-3.1221
C	-2.2657	-2.0150	-2.5384
C	-2.4743	-2.6781	-1.2894
C	0.6226	-0.0365	-3.4372
C	-0.5748	-0.6970	-3.7566
C	4.1033	-0.2577	-0.1288
C	3.8218	-1.0341	1.0636
C	3.0506	1.0647	-2.4150

C	3.4204	1.7955	-1.2691
C	3.9366	1.1290	-0.1189
C	-0.0543	1.6865	-3.0613
C	1.1500	2.3635	-2.8090
C	-2.5713	0.3407	-3.1345
C	-3.1045	-0.8306	-2.5621
C	-1.2469	2.1801	-2.3204
C	-2.5476	1.5361	-2.3483
C	1.7211	-2.2387	2.5625
C	2.2268	-1.0032	2.9371
C	3.3061	-0.3950	2.1903
C	3.3749	1.7826	1.0472
C	3.0552	1.0312	2.1652
C	-3.4707	-1.9260	-0.5536
C	-3.3882	-1.8141	0.8239
C	-2.2956	-2.4412	1.5413
C	-3.8452	-0.7705	-1.3452
C	0.2950	-2.4861	2.6116
C	-1.9417	-1.5972	2.6395
C	-0.6043	-1.5114	3.1093
C	1.3224	0.0409	3.3701
C	-0.0720	-0.1980	3.4964
C	1.8260	1.2893	2.8889
C	1.3700	3.1398	-1.5962

C	2.5378	2.8614	-0.8324
C	-1.0682	3.1826	-1.3404
C	0.2370	3.5306	-0.8779
C	-3.4175	1.6356	-1.2459
C	-4.0707	0.4591	-0.7224
C	-1.9724	3.2903	-0.2156
C	-3.1094	2.5090	-0.1480
C	2.4916	2.8388	0.5960
C	0.9553	2.3439	2.5113
C	1.2864	3.1288	1.3118
C	0.2115	3.6418	0.5535
C	-1.1606	3.5003	0.9655
C	-4.0393	0.5590	0.7242
C	-3.7037	-0.5627	1.4812
C	-3.4776	1.8474	1.0820
C	-1.4743	2.8210	2.1338
C	-2.6487	1.9775	2.1926
C	-2.8014	-0.4333	2.6043
C	-2.2945	0.8067	2.9611
C	-0.9122	0.9358	3.3739
C	-0.4093	2.1848	2.8766
C	2.2276	1.6545	-3.3948
C	-1.5633	0.2528	-4.1146

Table S15. Geometric coordinates of Y₃N@^{#22010}C₇₈

Atom	X (Å)	Y (Å)	Z (Å)
C	0.7754	2.0714	-2.8658
C	-0.2374	1.1465	-3.4114
C	-1.6376	1.4229	-3.1426
C	-2.6033	0.3793	-3.4126
C	-3.8861	0.3079	-2.7175
C	-4.2404	-1.0874	-2.5329
C	-4.5452	-1.6276	-1.2126
C	-3.6983	-2.8073	-1.0344
C	-3.2194	-3.2116	0.2658
C	-1.9735	-3.8784	0.3214
C	-1.1385	-3.8031	1.4921
C	0.2213	-3.9011	1.0642
C	1.2615	-3.2522	1.7671
C	2.4097	-2.8741	1.0283
C	3.1703	-1.7103	1.3883
C	3.7631	-1.1726	0.1836
C	3.8999	0.2511	-0.0132
C	3.8097	0.7606	-1.3740
C	2.9688	1.9328	-1.6162
C	2.1569	1.6714	-2.8020
C	0.3741	3.0464	-1.9134
C	1.1839	3.3543	-0.7480
C	2.4260	2.7143	-0.5299
C	2.7451	2.3257	0.8133
C	3.4281	1.0830	1.0628
C	2.8957	0.5347	2.2843
C	2.7333	-0.8653	2.4544

C	1.6282	-1.2883	3.2781
C	0.9089	-2.4756	2.9228
C	-0.4467	-2.3348	3.3548
C	-1.4969	-2.9809	2.6038
C	-2.7435	-2.3058	2.5455
C	-3.6042	-2.4297	1.4037
C	-4.2871	-1.1756	1.2192
C	-4.7015	-0.7220	-0.0838
C	-4.5651	0.6945	-0.3322
C	-4.1055	1.1870	-1.6263
C	-3.2166	2.2866	-1.3991
C	-2.0120	2.4506	-2.1704
C	-0.9883	3.2067	-1.5521
C	-1.0453	3.5860	-0.1621
C	0.2896	3.6372	0.3434
C	0.5832	3.2029	1.6720
C	1.8246	2.5522	1.8909
C	1.9198	1.4529	2.8326
C	0.8392	1.0497	3.7069
C	0.7266	-0.3829	3.9798
C	-0.5938	-1.0529	4.0397
C	-1.8354	-0.3070	3.8514
C	-2.8744	-0.9686	3.0914
C	-3.8122	-0.2721	2.2362
C	-3.6485	1.1130	1.9713
C	-4.0260	1.5821	0.6746
C	-3.2377	2.5813	0.0109
C	-2.1256	3.1798	0.6540

C	-1.8402	2.8062	2.0094
C	-0.5083	2.8122	2.5274
C	-0.4043	1.7991	3.5724
C	-1.7216	1.1343	3.6550
C	-2.5844	1.7788	2.6743
C	-2.1612	-1.0005	-3.6346
C	-3.1836	-1.8716	-3.1050
C	-2.8228	-2.9174	-2.1970
C	-1.4452	-3.3089	-2.0647
C	-1.1027	-3.9394	-0.8381
C	0.2379	-3.9699	-0.3766
C	1.2972	-3.4327	-1.1456
C	2.4620	-3.0298	-0.4028
C	3.3657	-2.0445	-0.9143
C	3.2108	-1.5490	-2.2334
C	3.5697	-0.1645	-2.4753
C	2.5541	0.3960	-3.3204
C	1.5516	-0.6053	-3.6047
C	0.1738	-0.2519	-3.6817
C	-0.7849	-1.3499	-3.5302
C	-0.4000	-2.5915	-2.8177
C	0.9818	-2.7597	-2.4068
C	1.9678	-1.8443	-2.9396
N	-0.3996	-0.2495	-0.1921
Y	-0.4257	0.0278	1.8488
Y	1.4834	-0.1268	-1.1153
Y	-2.2423	-0.6592	-1.1103

Table S16. Geometric coordinates of Y₃N@^{#31924}C₈₀

Atom	X (Å)	Y (Å)	Z (Å)
C	9.8306	7.5550	9.0030
C	9.8471	8.9319	8.5950
C	10.5411	9.0311	7.3355
C	10.9347	7.6927	6.9627
C	10.4967	6.7880	7.9898
C	10.0853	5.4616	7.6835
C	9.0484	4.8921	8.4719
C	8.3687	5.6614	9.4754
C	8.7239	7.0165	9.7178
C	7.6755	7.9058	10.1004
C	7.6968	9.2763	9.6849
C	8.7696	9.7991	8.8923
C	8.4741	10.8384	7.9312
C	9.2230	11.0507	6.7057
C	10.2136	10.0326	6.3647
C	10.3182	9.6353	4.9898
C	10.6866	8.2853	4.6304
C	10.9709	7.2898	5.6068
C	10.6343	5.9195	5.2921
C	10.2002	5.0163	6.3145
C	9.3423	4.0147	5.7182
C	8.2043	3.5741	6.5123
C	8.1112	3.9752	7.8875
C	6.8416	4.1948	8.5370
C	6.9946	5.2328	9.5294
C	5.9179	6.1113	9.9072
C	6.2997	7.4712	10.1931
C	5.4521	8.5983	9.8313

C	6.3424	9.7027	9.4965
C	6.0310	10.6522	8.4825
C	7.1160	11.2462	7.7230
C	6.9824	11.6988	6.3562
C	8.3020	11.6287	5.6911
C	8.3579	11.1176	4.2975
C	9.3924	10.1399	3.9834
C	9.1910	9.0489	3.0386
C	10.0036	7.9278	3.4236
C	9.6321	6.5641	3.1332
C	10.0444	5.5066	4.0385
C	9.2553	4.2735	4.2615
C	7.9423	4.1304	3.5830
C	6.8295	3.6619	4.4042
C	6.9690	3.3599	5.8267
C	5.7036	3.6112	6.4830
C	5.6205	4.0503	7.8421
C	4.5180	4.9093	8.2439
C	4.5912	5.8817	9.3300
C	3.6998	7.0227	8.9733
C	4.1702	8.4110	9.1829
C	3.9038	9.3797	8.1428
C	4.7798	10.5029	7.8410
C	4.6384	10.8505	6.4557
C	5.7286	11.3880	5.6871
C	5.8043	11.0097	4.3153
C	7.0922	10.8341	3.6514
C	6.9058	9.7560	2.6916
C	7.9446	8.8305	2.3892

C	7.5906	7.4833	2.0521
C	8.4237	6.3640	2.4078
C	7.5738	5.2011	2.6661
C	6.2058	5.6694	2.5001
C	5.1346	5.1649	3.3002
C	5.4616	4.1399	4.2367
C	4.7795	4.0815	5.4989
C	3.7510	5.0141	5.8491
C	3.6143	5.3989	7.2386
C	3.1301	6.6950	7.6532
C	2.8872	7.6865	6.6135
C	3.2386	9.0390	6.9038
C	3.6912	9.9382	5.8792
C	3.8183	9.5074	4.5293
C	4.8632	10.0865	3.7438
C	5.5432	9.3167	2.7489
C	5.1892	7.9534	2.5037
C	6.2282	7.0505	2.1176
C	4.0865	7.4171	3.2204
C	4.0527	6.0375	3.6094
C	3.3650	5.9571	4.8704
C	2.9502	7.2837	5.2486
C	3.4049	8.1848	4.2231
N	6.7540	7.5188	5.9069
Y	7.6862	9.3592	5.7814
Y	5.5941	7.2158	7.5870
Y	7.8026	5.9140	5.1421

Table S17. Geometric coordinates of INT1-Y₃N@C₇₈C

Atom	X (Å)	Y (Å)	Z (Å)
C	-1.7271	1.9043	-2.8768
C	-0.8063	2.8154	-2.1946
C	0.6052	2.7285	-2.4741
C	1.5041	3.4081	-1.5713
C	2.9053	3.0152	-1.4397
C	3.3136	3.2262	-0.0613
C	3.9056	2.1581	0.7438
C	3.1250	2.0975	1.9822
C	2.9369	0.8720	2.7145
C	1.7519	0.7482	3.4736
C	1.1707	-0.5444	3.7365
C	-0.2417	-0.3725	3.8629
C	-1.1572	-1.3803	3.4776
C	-2.4416	-0.9670	3.0373
C	-3.1431	-1.7095	2.0260
C	-3.9321	-0.7738	1.2675
C	-4.1220	-0.9193	-0.1363
C	-4.2657	0.2980	-0.9142
C	-3.5671	0.3663	-2.1789
C	-3.0424	1.7021	-2.3219
C	-1.1822	0.8217	-3.6168
C	-1.7599	-0.5063	-3.5556
C	-2.8930	-0.7678	-2.7525
C	-2.9522	-2.0148	-2.0570
C	-3.5333	-2.0763	-0.7461
C	-2.7778	-3.0337	0.0182
C	-2.5423	-2.8495	1.4071

C	-1.2923	-3.3623	1.9270
C	-0.6128	-2.5986	2.9394
C	0.7971	-2.7865	2.7844
C	1.7118	-1.7297	3.1614
C	2.9011	-1.6006	2.3962
C	3.5226	-0.3232	2.1904
C	4.1138	-0.3149	0.8743
C	4.2729	0.8981	0.1088
C	4.0469	0.7742	-1.3208
C	3.3266	1.8083	-2.0657
C	2.4650	1.1563	-3.0135
C	1.1312	1.6303	-3.2743
C	0.2205	0.6796	-3.7926
C	0.5283	-0.7286	-3.8346
C	-0.6898	-1.4585	-3.6590
C	-0.7100	-2.6693	-2.8991
C	-1.8629	-2.9437	-2.1142
C	-1.7468	-3.6109	-0.8277
C	-0.5118	-4.1721	-0.3229
C	-0.3017	-4.0903	1.1336
C	1.0251	-3.7093	1.6810
C	2.1623	-3.4352	0.8118
C	3.0885	-2.4029	1.2104
C	3.8150	-1.5887	0.2663
C	3.5604	-1.6949	-1.1273
C	3.6719	-0.4992	-1.9049
C	2.7412	-0.2535	-2.9693
C	1.7563	-1.2149	-3.3306

C	1.7469	-2.4678	-2.6384
C	0.5337	-3.1947	-2.4163
C	0.6517	-3.9405	-1.1691
C	1.9644	-3.5993	-0.6090
C	2.6280	-2.7043	-1.5373
C	1.0360	3.8465	-0.2461
C	2.1677	3.7290	0.6382
C	2.0218	3.0438	1.8760
C	0.7119	2.7740	2.3995
C	0.6654	1.7019	3.3377
C	-0.5391	1.0101	3.6156
C	-1.7470	1.4247	3.0340
C	-2.7616	0.4264	2.8764
C	-3.7334	0.5451	1.8288
C	-3.8906	1.7540	1.0906
C	-4.2736	1.6370	-0.3183
C	-3.5356	2.5054	-1.2327
C	-2.6716	3.5160	-0.6665
C	-1.2739	3.4784	-0.9594
C	-0.3080	3.6565	0.2010
C	-0.5066	3.1615	1.6420
C	-1.7698	2.5886	2.1673
C	-3.0008	2.8590	1.4479
C	-2.8748	4.0593	0.6646
N	0.0108	0.1245	-0.0445
Y	0.1770	-1.9107	0.2384
Y	1.7293	1.3272	-0.0845
Y	-1.8641	1.0305	-0.1699

Table S18. Geometric coordinates of TS-Y₃N@C₇₈C

Atom	X (Å)	Y (Å)	Z (Å)
C	2.2563	-2.4893	-2.1179
C	1.3240	-3.3309	-1.3475
C	-0.0938	-3.3756	-1.6617
C	-1.0116	-3.7769	-0.6153
C	-2.4479	-3.5059	-0.7599
C	-3.0390	-3.3624	0.5538
C	-3.8423	-2.1948	0.9388
C	-3.2653	-1.7043	2.1938
C	-3.2454	-0.3048	2.5538
C	-2.1968	0.1566	3.3915
C	-1.7137	1.5128	3.3109
C	-0.3212	1.5104	3.6513
C	0.5950	2.4234	3.0757
C	1.9440	1.9951	2.9102
C	2.7282	2.4688	1.8012
C	3.6407	1.4187	1.4363
C	3.9958	1.1846	0.0828
C	4.2729	-0.1777	-0.3014
C	3.8214	-0.6445	-1.5859
C	3.4649	-2.0370	-1.4608
C	1.7155	-1.6750	-3.1303
C	2.1891	-0.3302	-3.3659
C	3.1809	0.2315	-2.5285
C	3.0666	1.6150	-2.1918
C	3.4580	2.0812	-0.8946
C	2.5720	3.1560	-0.5301
C	2.1674	3.3537	0.8227

C	0.8476	3.9168	1.0420
C	0.0749	3.3926	2.1449
C	-1.3095	3.3857	1.7737
C	-2.2220	2.4157	2.3391
C	-3.2899	1.9607	1.5156
C	-3.8068	0.6248	1.6265
C	-4.2087	0.1806	0.3099
C	-4.2034	-1.2110	-0.0796
C	-3.7775	-1.4745	-1.4445
C	-2.8847	-2.5971	-1.7665
C	-1.9648	-2.1586	-2.7740
C	-0.5906	-2.5711	-2.7666
C	0.3218	-1.7195	-3.4484
C	-0.0619	-0.4150	-3.9117
C	1.0822	0.4495	-3.8329
C	0.9333	1.8156	-3.4434
C	1.9556	2.4005	-2.6415
C	1.6443	3.3955	-1.6258
C	0.3208	3.9522	-1.4361
C	-0.0727	4.2775	-0.0486
C	-1.4245	3.9078	0.4270
C	-2.4127	3.2824	-0.4359
C	-3.3572	2.3621	0.1367
C	-3.8993	1.2536	-0.6065
C	-3.4694	0.9859	-1.9332
C	-3.4075	-0.3872	-2.3309
C	-2.3333	-0.8291	-3.1732
C	-1.3730	0.0786	-3.6986

C	-1.5262	1.4701	-3.4124
C	-0.3894	2.3299	-3.2681
C	-0.6977	3.3512	-2.2810
C	-2.0446	3.0573	-1.8004
C	-2.5520	1.9158	-2.5210
C	-0.7013	-3.7874	0.8589
C	-1.9751	-3.5197	1.5014
C	-2.1010	-2.5185	2.5067
C	-0.9309	-1.9756	3.1164
C	-1.0613	-0.6851	3.6990
C	0.0696	0.1492	3.8914
C	1.3679	-0.3204	3.5949
C	2.3441	0.6498	3.2052
C	3.4279	0.2983	2.3242
C	3.6980	-1.0534	1.9566
C	4.2594	-1.3015	0.6312
C	3.8367	-2.4899	-0.1268
C	2.9648	-3.4456	0.5118
C	1.7425	-3.8317	-0.0921
C	0.5305	-3.3870	1.5061
C	0.3792	-2.4349	2.6698
C	1.5275	-1.6653	3.1130
C	2.7805	-2.0729	2.4880
C	2.6252	-3.3344	1.8871
N	0.0225	-0.1504	-0.0490
Y	-0.0741	1.9001	-0.2191
Y	-1.6827	-1.3591	0.1531
Y	1.7656	-1.2350	0.3052

Table S19. Geometric coordinates of INT2-Y₃N@C₇₈C

Atom	X (Å)	Y (Å)	Z (Å)
C	-2.8511	-0.0668	-2.9378
C	-1.8813	0.8767	-3.5248
C	-0.5019	0.4897	-3.7665
C	0.5597	1.4699	-3.5134
C	1.9564	1.0110	-3.6114
C	2.8311	1.9120	-2.9051
C	3.8002	1.4565	-1.8968
C	3.5761	2.2960	-0.7127
C	3.7039	1.7869	0.6436
C	2.8971	2.3595	1.6673
C	2.4538	1.5859	2.8067
C	1.1710	2.0839	3.2098
C	0.1826	1.2292	3.7673
C	-1.1843	1.5365	3.5178
C	-2.1648	0.4961	3.4107
C	-3.1598	0.9322	2.4591
C	-3.8136	0.0137	1.5948
C	-4.2417	0.4926	0.2932
C	-4.1698	-0.3812	-0.8608
C	-3.8823	0.4293	-2.0363
C	-2.4561	-1.4129	-2.8374
C	-2.8916	-2.2724	-1.7643
C	-3.6698	-1.7369	-0.7078
C	-3.3990	-2.2327	0.6078
C	-3.4752	-1.3695	1.7488
C	-2.4852	-1.8061	2.6988
C	-1.7938	-0.8794	3.5272

C	-0.4349	-1.2217	3.9067
C	0.5321	-0.1530	3.9711
C	1.8096	-0.6673	3.5701
C	2.7723	0.2087	2.9310
C	3.6112	-0.3577	1.9322
C	4.0743	0.4142	0.8082
C	4.1541	-0.4599	-0.3378
C	3.9802	0.0169	-1.6922
C	3.2498	-0.8784	-2.5657
C	2.2440	-0.3808	-3.5079
C	1.1885	-1.3382	-3.5770
C	-0.1671	-0.9265	-3.7281
C	-1.1547	-1.8416	-3.2604
C	-0.8046	-2.9942	-2.4770
C	-1.8611	-3.2433	-1.5357
C	-1.5654	-3.6970	-0.2153
C	-2.3664	-3.2032	0.8491
C	-1.7967	-2.9695	2.1663
C	-0.4459	-3.3430	2.5393
C	0.2470	-2.4606	3.5004
C	1.6677	-2.0824	3.2677
C	2.4210	-2.5813	2.1217
C	3.3963	-1.7142	1.5040
C	3.7133	-1.7674	0.0978
C	3.0028	-2.6329	-0.7715
C	2.7850	-2.1739	-2.1080
C	1.5449	-2.4670	-2.7623
C	0.5481	-3.2708	-2.1495

C	0.8263	-3.8287	-0.8610
C	-0.2100	-4.0353	0.1056
C	0.3491	-3.8685	1.4376
C	1.7561	-3.5093	1.2482
C	2.0354	-3.5063	-0.1723
C	0.5785	2.7438	-2.6447
C	1.9962	2.9338	-2.3318
C	2.4821	3.2116	-1.0044
C	1.5670	3.6315	-0.0009
C	1.8499	3.2957	1.3524
C	0.8026	3.1394	2.3101
C	-0.5534	3.3513	1.9461
C	-1.5561	2.6008	2.6273
C	-2.7896	2.2448	1.9860
C	-3.1145	2.6854	0.6585
C	-3.9922	1.8589	-0.1533
C	-3.8328	1.8371	-1.6135
C	-2.8014	2.6221	-2.2698
C	-2.1946	2.2462	-3.5105
C	-0.3428	3.3600	-1.6821
C	0.1984	3.7866	-0.3961
C	-0.8300	3.7371	0.6010
C	-2.0688	3.4068	-0.0286
C	-1.8266	3.2685	-1.4493
N	-0.0023	0.1488	0.0045
Y	0.2517	-1.3114	1.4237
Y	1.6051	0.7440	-1.1761
Y	-1.8538	0.7905	-0.6507

Table S20. Geometric coordinates of INT-Y₃N@C₇₉C

Atom	X (Å)	Y (Å)	Z (Å)
C	-3.6773	0.6358	-1.7067
C	-3.2233	1.9891	-1.4255
C	-1.9610	2.5115	-1.8628
C	-1.1179	3.4268	-1.0521
C	0.1870	3.8362	-1.5992
C	1.0541	4.2949	-0.5410
C	2.4166	3.7718	-0.3388
C	2.4945	3.3807	1.0753
C	3.2485	2.2209	1.5253
C	2.7944	1.5177	2.6772
C	3.0132	0.0950	2.8343
C	1.9113	-0.4442	3.5754
C	1.4360	-1.7650	3.3469
C	0.0487	-2.0164	3.5337
C	-0.6377	-2.9969	2.7419
C	-1.9924	-2.5360	2.5541
C	-2.7068	-2.7914	1.3519
C	-3.6954	-1.8179	0.9256
C	-3.9167	-1.5352	-0.4810
C	-4.3300	-0.1390	-0.6309
C	-2.9201	-0.0793	-2.6606
C	-2.6815	-1.4994	-2.6001
C	-3.0944	-2.2330	-1.4611
C	-2.2247	-3.2884	-1.0311
C	-2.0397	-3.5746	0.3609
C	-0.6872	-4.0332	0.5449
C	0.0475	-3.7326	1.7267
C	1.4876	-3.5938	1.5961

C	2.1396	-2.5735	2.3841
C	3.2429	-2.0477	1.6319
C	3.6564	-0.6691	1.8250
C	4.1419	0.0352	0.6894
C	3.9477	1.4556	0.5390
C	3.7654	1.7392	-0.8641
C	2.9736	2.8569	-1.3324
C	2.1725	2.5880	-2.5111
C	0.7970	3.0654	-2.6280
C	0.0376	2.0701	-3.3173
C	-1.3208	1.8109	-2.9837
C	-1.8184	0.5276	-3.3431
C	-0.9338	-0.5290	-3.7711
C	-1.4539	-1.7749	-3.2873
C	-0.5732	-2.8002	-2.8278
C	-0.9878	-3.5703	-1.7094
C	-0.0195	-4.0606	-0.7423
C	1.4153	-3.9280	-0.8999
C	2.2156	-3.7543	0.3288
C	3.3149	-2.7488	0.3594
C	3.6488	-1.9398	-0.8099
C	4.0849	-0.5780	-0.6102
C	3.8313	0.4764	-1.5639
C	3.0463	0.2329	-2.7199
C	2.2267	1.3049	-3.1891
C	0.9278	1.0191	-3.7194
C	0.4594	-0.3129	-3.8813
C	1.3395	-1.3852	-3.5268
C	0.8367	-2.6146	-2.9937

C	1.8136	-3.1527	-2.0623
C	2.9162	-2.1933	-2.0202
C	2.6127	-1.1174	-2.9388
C	-1.0336	3.6251	0.4537
C	0.3126	4.1547	0.6799
C	1.2005	3.6408	1.6894
C	0.6753	2.8170	2.7221
C	1.5278	1.8267	3.2876
C	0.9975	0.6268	3.8528
C	-0.4036	0.4012	3.8907
C	-0.8665	-0.9468	3.8173
C	-2.1339	-1.2742	3.2356
C	-3.0167	-0.2602	2.7420
C	-3.9231	-0.5921	1.6656
C	-4.3752	0.4428	0.7339
C	-3.8955	1.7979	0.8891
C	-3.9940	2.6407	-0.3073
C	-1.6233	2.9547	1.6069
C	-0.7404	2.5807	2.7049
C	-1.2580	1.4164	3.3677
C	-2.5187	1.0884	2.7969
C	-2.8217	2.0561	1.7649
C	-4.5457	3.7113	-0.7995
N	0.0292	0.0379	0.1429
Y	1.1735	-1.6568	-0.0502
Y	0.8883	1.9017	-0.2426
Y	-2.0333	0.0555	0.2269

Table S21. Geometric coordinates of TS-Y₃N@C₇₉C

Atom	X (Å)	Y (Å)	Z (Å)
C	-3.1998	1.6732	-2.0012
C	-2.4289	2.8104	-1.5553
C	-1.0843	2.9866	-1.9109
C	-0.3147	3.8129	-0.9003
C	1.2104	3.8151	-1.2438
C	2.0315	3.8890	-0.0712
C	3.2348	3.0678	0.2051
C	3.0779	2.5694	1.5884
C	3.4630	1.2205	1.9786
C	2.7368	0.5634	3.0198
C	2.5788	-0.8731	3.0499
C	1.3079	-1.1700	3.6448
C	0.5449	-2.3022	3.2472
C	-0.8721	-2.2008	3.2922
C	-1.6883	-2.9037	2.3464
C	-2.8533	-2.0896	2.0905
C	-3.4590	-2.0492	0.8111
C	-4.1003	-0.8142	0.3992
C	-4.0831	-0.4023	-0.9868
C	-4.1042	1.0504	-1.0404
C	-2.5800	0.8647	-2.9867
C	-2.7114	-0.5739	-3.0191
C	-3.3902	-1.2304	-1.9685
C	-2.8685	-2.5032	-1.5626
C	-2.9111	-2.9140	-0.1926
C	-1.7549	-3.7321	0.0606
C	-1.1031	-3.7154	1.3264
C	0.3295	-3.9433	1.3310

C	1.1220	-3.1826	2.2658
C	2.3900	-2.8951	1.6623
C	3.1128	-1.6957	2.0251
C	3.8767	-1.0564	1.0093
C	4.0506	0.3752	0.9800
C	4.1081	0.7995	-0.3991
C	3.6607	2.1175	-0.8216
C	2.9255	2.1279	-2.0652
C	1.7116	2.9502	-2.2629
C	0.8700	2.2342	-3.1774
C	-0.5354	2.2726	-3.0079
C	-1.3047	1.1992	-3.5373
C	-0.6610	-0.0156	-3.9534
C	-1.5237	-1.1161	-3.6192
C	-0.9744	-2.3510	-3.1661
C	-1.6852	-3.0599	-2.1588
C	-0.9814	-3.8580	-1.1664
C	0.4512	-4.1006	-1.1944
C	1.1277	-4.1965	0.1177
C	2.4184	-3.4933	0.3383
C	3.0715	-2.7222	-0.7103
C	3.8119	-1.5372	-0.3408
C	3.9316	-0.3877	-1.2052
C	3.2395	-0.3470	-2.4420
C	2.7579	0.9313	-2.8639
C	1.5086	1.0206	-3.5629
C	0.7501	-0.1426	-3.9016
C	1.2911	-1.4193	-3.5543
C	0.4487	-2.5211	-3.1896

C	1.1569	-3.3647	-2.2386
C	2.4467	-2.7098	-2.0014
C	2.5193	-1.5249	-2.8317
C	-0.2089	3.5577	0.7431
C	1.1640	3.8002	1.0723
C	1.8224	3.0771	2.1255
C	1.0197	2.3479	3.0542
C	1.5376	1.1329	3.5761
C	0.6659	0.0693	3.9677
C	-0.7498	0.2064	3.8865
C	-1.5200	-0.9596	3.6165
C	-2.7563	-0.8924	2.8874
C	-3.3079	0.3524	2.4439
C	-4.1002	0.3798	1.2266
C	-4.1448	1.5685	0.3455
C	-3.3338	2.7500	0.6695
C	-2.7195	3.5892	-0.3736
C	-1.0464	3.1083	1.8126
C	-0.4026	2.4874	2.9550
C	-1.2735	1.4541	3.4361
C	-2.5191	1.5225	2.7234
C	-2.4500	2.6043	1.7796
C	-1.7984	4.6498	-0.0718
N	0.0109	-0.0026	0.2403
Y	0.6149	-1.9108	-0.2221
Y	1.3898	1.5437	0.0530
Y	-1.9432	0.6486	0.0880

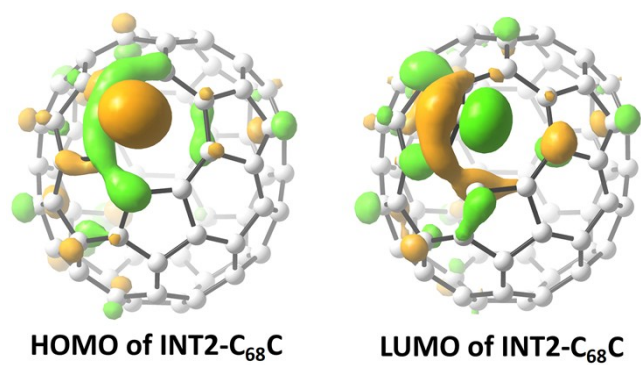


Fig. S1 Frontier orbitals of INT2-C₆₈C.

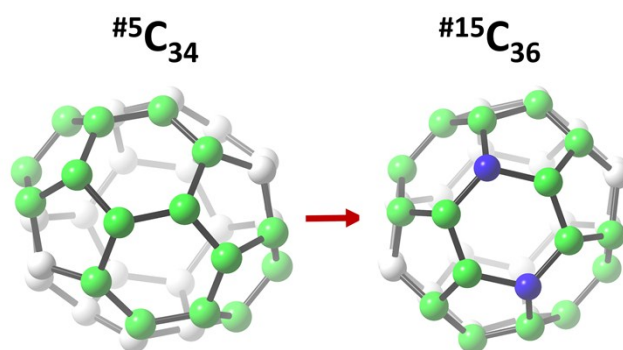


Fig. S2 Fullerene growth via a modified-SDD addition from #5C₃₄ to #15C₃₆. The SDD addition patch is colored in green and the two adatoms are colored in blue.

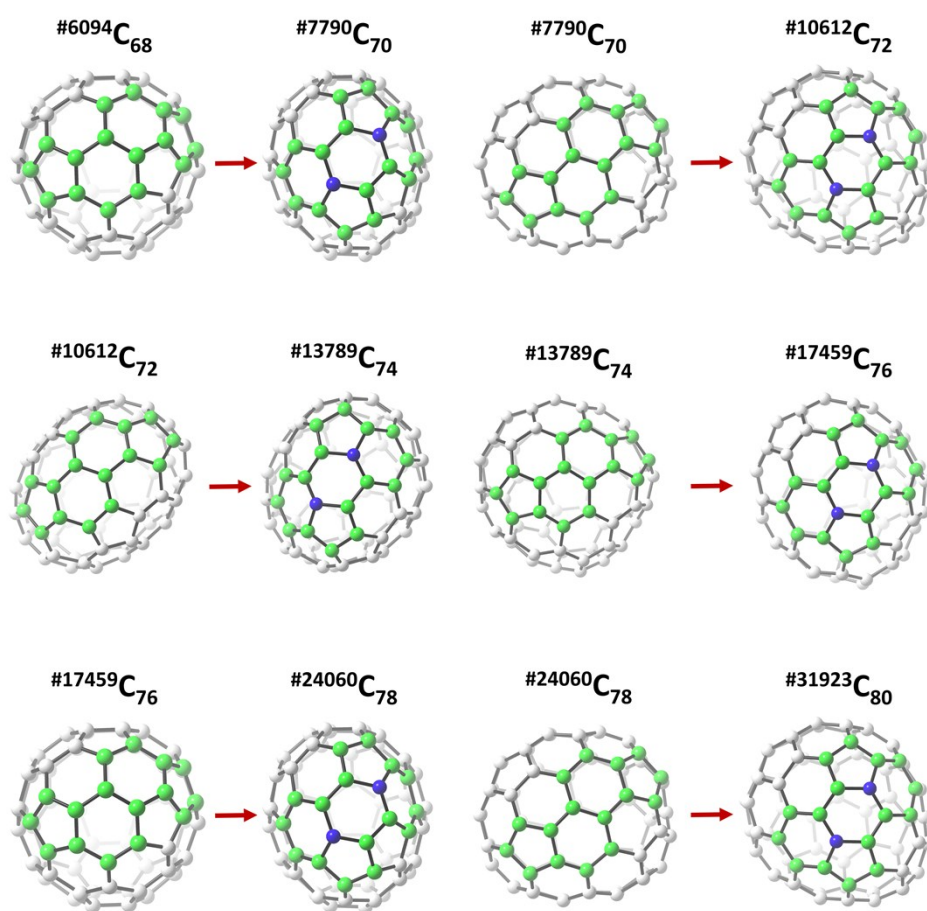


Fig. S2 Fullerene growth via modified-SDD additions from $\#6094\text{C}_{68}$ to $\#31923\text{C}_{80}$. The SDD addition patch is colored in green and the two adatoms are colored in blue. Each intermediate along the growth pathway is drawn from two views to show the reaction site as a reactant and a product.