

SWCNT Growth from Chiral Carbon Nanorings: Prediction of Chirality and Diameter Influence on Growth Rates

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Supporting Information

Movies

Movie S1: Computed QM/MD trajectory of (6,5)-SWCNT growth from a [4]CPPN precursor including the manual removal of hydrogens. Cyan and grey spheres represent carbon and hydrogen atoms, respectively. Magenta spheres represent the carbon atoms of the most recently added C₂H radical. The total length of the movie is 240 ps; each frame is separated by 0.8 ps.

Movie S2. Computed QM/MD trajectory of (10,1)-SWCNT growth from a [0]CPPD precursor including the manual removal of hydrogens. Cyan and grey spheres represent carbon and hydrogen atoms, respectively. Magenta spheres represent the carbon atoms of the most recently added C₂H radical. The total length of the movie is 240 ps; each frame is separated by 0.8 ps.

Movie S3. Computed QM/MD trajectory of (4,3)-SWCNT growth from a [2]CPPN precursor including the manual removal of hydrogens. Cyan and grey spheres represent carbon and hydrogen atoms, respectively. Magenta spheres represent the carbon atoms of the most recently added C₂H radical. The total length of the movie is 240 ps; each frame is separated by 0.8 ps.

Figures

Figure S1. Snapshots of QM/MD simulations of (4,3)- and (6,1)-SWCNTs hydrocarbon organic model systems. Snapshots times given with respect to the beginning of the simulation. Pink spheres represent C for the initial model system, Cyan ones from supplied C₂H radicals, Dark green ones from latest C₂H radical.

Figure S2. (a) Reaction mechanism for hexagon addition *via* C₂H₂ insertion to [*n*]CPP radical precursors (R). (b) $\Delta G^\ddagger(\text{TS1})$, (c) $\Delta G(\text{INT})$ (d) $\Delta G^\ddagger(\text{TS2})$ and (e) $\Delta G(\text{P})$ for [*n*]CPP precursors. All data computed using B3LYP/6-31G(d); Gibbs free energies calculated at 500 K.

S1. DFTB energies (in Hartree) and cartesian coordinates (in Å) for the organic templates in Figure 1.

S2. Complete citation for references 11, 19, and 54.

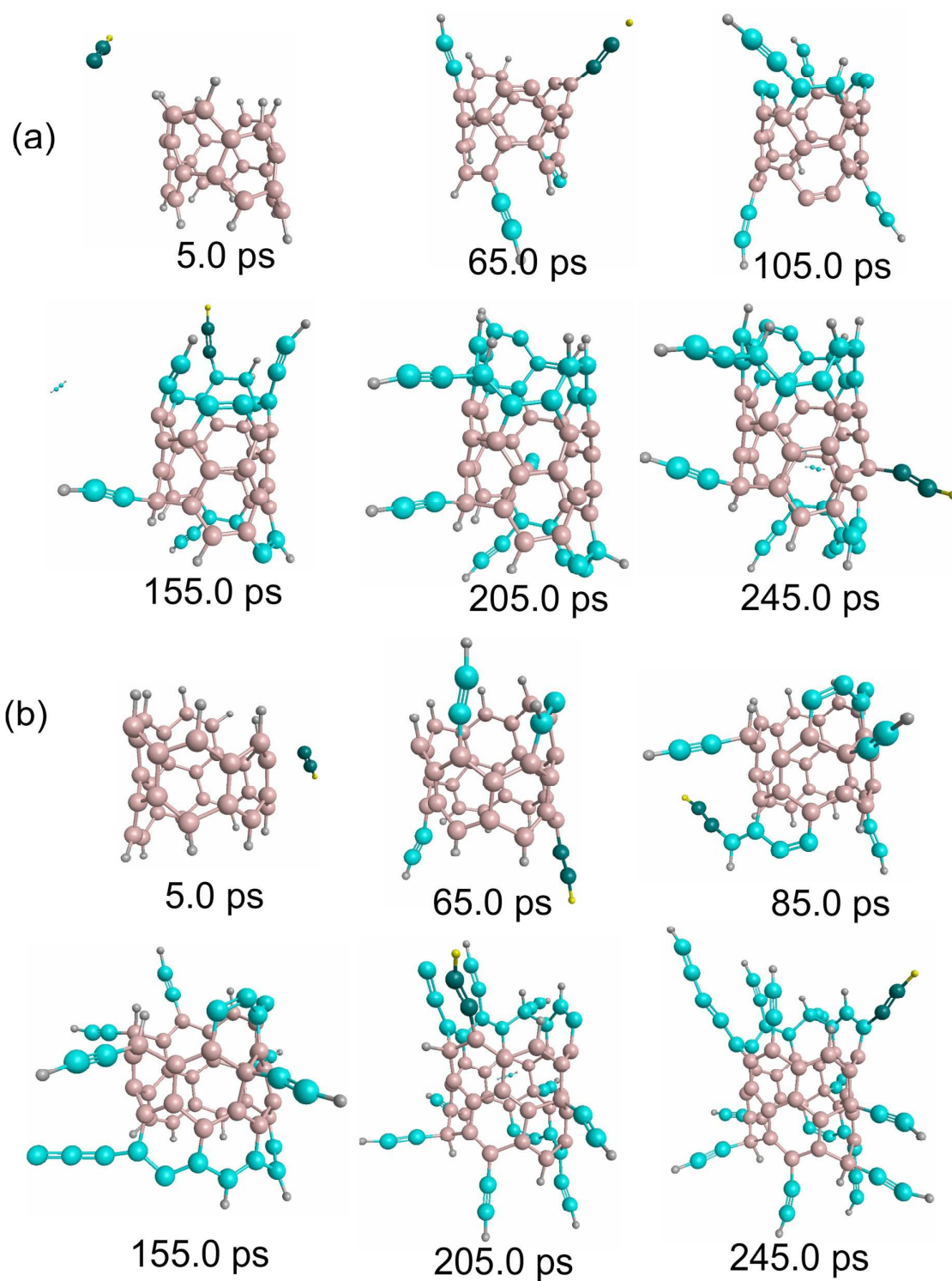


Figure S1. Snapshots of QM/MD simulations of (4,3)- and (6,1)-SWCNTs hydrocarbon organic model systems. Snapshots times given with respect to the beginning of the simulation. Pink spheres represent C for the initial model system, Cyan ones from supplied C_2H radicals, Dark green ones from latest C_2H radical.

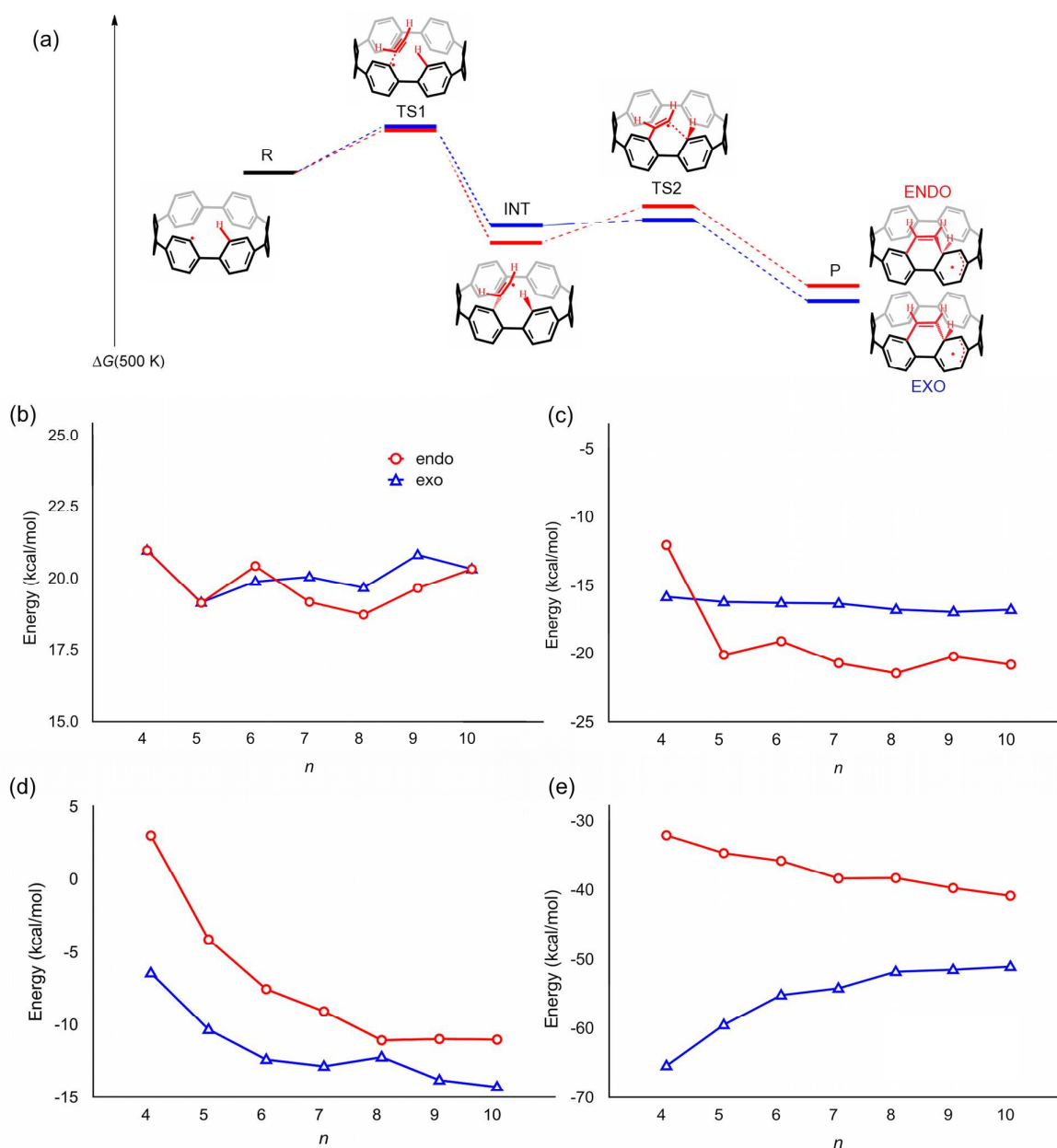


Figure S2. (a) Reaction mechanism for hexagon addition *via* C_2H_2 insertion to $[n]$ CPP radical precursors (R). (b) $\Delta G^\ddagger(TS1)$, (c) $\Delta G(INT)$ (d) $\Delta G^\ddagger(TS2)$ and (e) $\Delta G(P)$ for $[n]$ CPP precursors. All data computed using B3LYP/6-31G(d); Gibbs free energies calculated at 500 K.

S1. DFTB energies (in Hartree) and cartesian coordinates (in Å) for the organic templates in Figure 1.

[6] CPP:	Total Energy:	-70.9021250837
C	3.65788515	1.20852300
C	3.01766993	2.44195821
C	0.72860156	4.23998144
C	-0.66049994	4.30295206
C	-3.10100041	2.71756363
C	-3.84940081	1.54661066
C	-4.26156168	-1.33327624
C	-3.62137882	-2.56756304
C	-1.02905472	-3.88868457
C	0.35915106	-3.95142788
C	3.06047678	-2.86990419
C	3.80898931	-1.69804624
H	4.21314021	-1.33307860
H	3.76304294	0.67304258
H	2.64068669	2.83458149
H	1.26058917	4.35924327
H	-1.17982606	4.47016782
H	-2.68961578	3.07404789
H	-4.00138119	1.02213412
H	-4.63091023	-0.93314599
H	-3.50641150	-3.10160137
H	-1.54460671	-3.71171347
H	0.88821888	-3.82138391
H	2.89849906	-3.39206919
C	3.92033152	-0.90748364
C	3.98666192	0.56320967
C	2.67864565	3.08425026
C	1.43811094	3.87703774
C	-1.39940895	4.00549596
C	-2.70632614	3.32765284
C	-4.23557563	0.93417937
C	-4.30187999	-0.53641529
C	-2.99389742	-3.05755699
C	-1.75330110	-3.85031266
C	1.08414818	-3.97883439
C	2.39105705	-3.30094125
C	2.78576248	-2.69084484
C	3.53416475	-1.51992994
C	3.94627304	1.36001732
C	3.30604418	2.59431278
C	0.71392977	3.91543137
C	-0.67429248	3.97809402
C	-3.37578620	2.89659256
C	-4.12430432	1.72471649
C	-3.97308131	-1.18176928

C	-3.33290888	-2.41525270	1.24969845
C	-1.04382553	-4.21321028	1.13813321
C	0.34529536	-4.27626804	1.13785223
H	0.86457661	-4.44346431	2.09183804
H	2.37438581	-3.04729394	2.20293714
H	3.68619760	-0.99542917	2.20048172
H	4.31554925	0.95978460	2.08606981
H	3.19111782	3.12824631	2.08380514
H	1.22938060	3.73850026	2.19587369
H	-1.20348138	3.84796763	2.19619597
H	-3.21379144	3.41884115	2.08441954
H	-4.52850144	1.35988100	2.08722261
H	-4.07819484	-0.64626845	2.20215799
H	-2.95591597	-2.80789951	2.20406859
H	-1.57582443	-4.33249208	2.09236051

Cyclooctacene: Total Energy: -60.9079162270

C	2.23671355	-2.22128469	1.49751579
C	3.16881448	0.03430740	1.45716636
C	-0.01783397	-3.15637602	1.48913648
C	2.23309771	2.28773022	1.39210908
C	-2.27217638	-2.22210327	1.43615473
C	-0.02123265	3.22197651	1.33917682
C	-3.20630475	0.03194006	1.37020200
C	-2.27574970	2.28755674	1.32983588
C	2.90566006	-1.18954330	0.79313478
C	1.19900186	-2.89870742	0.81025945
C	2.90377154	1.22536956	0.73668671
C	-1.21606762	-2.89938730	0.77747650
C	1.19578199	2.93249697	0.67358707
C	-2.92320670	-1.19143657	0.71362677
C	-1.21933366	2.93264962	0.64005473
C	-2.92576383	1.22360595	0.65650814
C	2.92482493	-1.22335188	-0.65725971
C	1.21863662	-2.93293829	-0.64005829
C	2.92351069	1.19163606	-0.71359524
C	-1.19627079	-2.93334252	-0.67284127
C	1.21598119	2.89911769	-0.77680329
C	-2.90341641	-1.22529531	-0.73671428
C	-1.19916891	2.89863757	-0.81026086
C	-2.90590792	1.18967421	-0.79380938
C	3.20617356	-0.03168024	-1.37055484
C	2.27443979	-2.28731108	-1.33025127
C	0.02047778	-3.22307721	-1.33877072
C	2.27253559	2.22260494	-1.43560384
C	-2.23301005	-2.28800754	-1.39175554

C	0.01797010	3.15655616	-1.48858421
C	-3.16820386	-0.03440671	-1.45771250
C	-2.23648563	2.22125367	-1.49806760
H	2.18862722	-2.16207721	2.59624180
H	3.10650395	0.06020119	2.55637584
H	2.18341117	2.27888286	2.49226009
H	-0.03277154	-3.08203918	2.58788848
H	-2.25299347	-2.16235862	2.53564610
H	-0.03637934	3.19953397	2.44011273
H	-3.17185237	0.05817077	2.47070723
H	-2.25729452	2.27900628	2.43092724
H	2.25528949	-2.27907793	-2.43132228
H	3.17226893	-0.05751165	-2.47103824
H	0.03490814	-3.20090220	-2.43973261
H	2.25426983	2.16328363	-2.53513127
H	-2.18265431	-2.27905401	-2.49192356
H	0.03333736	3.08379279	-2.58744135
H	-3.10494774	-0.05995151	-2.55687857
H	-2.18698240	2.16123681	-2.59668104

[2]CPPN:	Total	Energy:	-53.2970443517
C	-2.44397101	8.53132070	0.02755422
C	-2.06823972	8.64663910	1.33668647
C	-2.11158631	11.08743620	1.17150074
C	-2.42620175	10.96799939	-0.22107830
C	-1.74292108	12.36471487	1.74292035
C	-1.58815575	9.92395324	1.81802440
C	-2.28299406	9.68432490	-0.83437571
C	-2.25952902	12.11504594	-1.08700206
C	-0.54186976	12.48068611	2.38507836
C	-0.29271774	10.04408493	2.41797857
C	-1.44427337	9.57606428	-1.98751602
C	-1.39129859	12.01027347	-2.13973681
C	0.33575986	11.32838677	2.40765689
C	-0.86442304	8.29534519	-2.36128291
C	0.58995359	8.89794866	2.43599087
C	-0.72796523	10.74834686	-2.37911800
C	1.63916265	11.43828398	1.82962703
C	0.49063391	8.18996038	-2.44140436
C	1.80129702	9.00428339	1.80801922
C	0.71004988	10.64898359	-2.35134588
C	2.12517248	12.71980024	1.34215179
C	2.17340712	10.26695667	1.21058548
C	1.27052573	9.35530489	-2.05385899
C	1.47889212	11.78367529	-1.95512252
C	2.44802042	10.36759387	-0.20117578

C	2.48790677	12.82648108	0.03418869
C	2.22293706	9.23331291	-1.03679034
C	2.27363069	11.66154191	-0.81062742
H	1.16624460	12.79206411	-2.26575962
H	2.46192722	8.22479030	-0.66663841
H	2.40572363	8.10471589	1.62146823
H	0.21574676	7.91263454	2.74914794
H	-1.98449112	7.75108245	1.96911034
H	-2.65702668	7.54230988	-0.40314494
H	-1.50386631	7.40511068	-2.44931176
H	0.97756764	7.21375028	-2.57710621
H	-1.08287791	12.91053505	-2.69083435
H	-2.64513715	13.09979733	-0.78608193
H	-2.34461934	13.25990152	1.52915410
H	-0.16644455	13.46980588	2.68457064
H	2.07628933	13.60951097	1.98656224
H	2.72212902	13.80319731	-0.41271027

[0]CPPH: Total	Energy:	-60.1494486130
H	2.18337261	-8.30264058
H	2.44422961	-14.27251905
H	0.18427624	-15.17810322
C	1.57908398	-13.59534714
C	1.75797479	-12.19850832
C	2.08879813	-9.39020840
C	0.92296371	-9.87905741
C	0.71450603	-11.30785103
H	-0.04295757	-7.92248471
C	0.32830626	-14.09818753
C	2.52803928	-11.69892410
C	2.60311296	-10.26143746
H	2.54808174	-13.62247732
C	-0.20839813	-9.01025102
C	-0.61287793	-11.83143913
C	2.62171372	-12.53212956
C	-0.81039716	-13.25523537
H	2.59665199	-8.63707121
C	2.65948583	-9.73148568
C	-1.42663004	-9.52389523
C	-1.61197744	-10.94772140
C	-1.89997548	-13.76902507
C	2.15270591	-11.98925640
H	-1.96372286	-14.85693828
C	2.08022246	-10.54733598
H	-2.35321767	-7.60116369
C	-2.31759641	-8.68122104

C	-2.41393895	-11.47187087	0.85618116
C	1.31566389	-12.79921707	-2.23292663
C	-2.47931877	-12.90077116	0.64725973
H	1.37841179	-13.89394833	-2.12675521
C	1.05387956	-9.98413541	-2.36871179
C	-2.83598666	-9.18476231	0.09395648
C	-2.70052994	-10.58184296	-0.22255214
C	-2.64710905	-13.39047833	-0.66650263
C	0.06870187	-12.23579780	-2.60233709
C	-0.09314003	-10.79378044	-2.57620018
H	-2.58151885	-14.47821340	-0.82923484
C	-2.23591141	-11.08249889	-1.50250277
C	-1.09207290	-13.05114494	-2.48283026
C	-2.12359496	-12.52017898	-1.67462925
C	-1.36572073	-10.25019505	-2.24155365
H	-0.96316897	-14.14561841	-2.49738386
H	-3.30373036	-8.50793842	-0.63553468
H	-1.43465391	-9.15973851	-2.10207082
H	0.93146580	-8.88931243	-2.35859820

[4]CPPN:	Total	Energy:	-84.0030268797
C	0.06083660	-0.05877353	-0.08996535
C	2.50404138	-0.00978772	-0.06310183
C	1.27540299	0.70408678	-0.05058336
C	3.71565321	0.75268191	-0.13686232
C	0.06263297	-1.37843505	0.28166402
C	2.50689204	-1.38788324	0.35849409
C	1.27686404	-1.99463474	0.73593579
C	1.28194840	2.08507192	0.35611079
C	3.72148645	2.07737540	0.22132135
C	3.71782942	-2.03387482	0.76615738
C	2.51856302	2.69893814	0.69332267
C	0.07645373	2.73400804	0.78391020
C	1.26673454	-2.94021271	1.81811771
C	3.70526258	-2.91270505	1.82262121
C	0.03082143	-3.34165637	2.44370852
C	2.48108165	-3.20800336	2.50192256
C	2.55121140	3.66147515	1.76424049
C	0.10917863	3.62445327	1.82691864
C	3.78665837	4.07544957	2.36263788
C	1.35052232	3.93094534	2.47578845
C	-0.01907671	-3.55377970	3.79187183
C	2.43871762	-3.38244050	3.93993027
C	1.16093931	-3.33025307	4.58907157
C	3.85463333	4.31499921	3.71163917
C	1.42363388	4.14611265	3.89800431

C	3.58495336	-3.19582733	4.74232633
C	2.69457896	4.12530897	4.53360110
C	0.26172170	4.00796628	4.72686465
C	1.05156478	-2.79650831	5.88326921
C	3.46948097	-2.54973742	5.98375788
C	2.17550228	-2.19709976	6.49154539
C	2.80622512	3.56235061	5.85398048
C	0.36971646	3.44340148	5.97292942
C	4.63041792	-1.97484868	6.61580271
C	1.64603918	3.01048094	6.46126074
C	4.08066636	3.21629759	6.41475350
C	2.05817407	-0.98572614	7.27820479
C	4.50603749	-0.80925324	7.31652968
C	0.78543687	-0.38479180	7.53618501
C	1.78259199	1.81254436	7.25067581
C	3.21464438	-0.18333090	7.45913458
C	4.21100780	2.09391854	7.19123838
C	0.65138806	0.98285944	7.53664997
C	3.07600032	1.24673373	7.42470578
H	4.97794266	3.78054843	6.12506655
H	5.21122663	1.77175388	7.51228756
H	4.83033320	4.51086021	4.17742005
H	4.70874016	4.08446522	1.76514978
H	5.40458159	-0.29305263	7.68221546
H	5.62413404	-2.39197409	6.39892120
H	4.67721218	2.61596478	0.28210902
H	0.04502230	-2.62796506	6.29250169
H	4.58880813	-3.31432125	4.30957363
H	4.66656656	0.24938673	-0.36001185
H	4.65744090	-3.28730783	2.22322475
H	4.67964539	-1.71753838	0.33968228
H	-0.89401223	0.44223804	-0.30104534
H	-0.89101388	-1.91759595	0.36558097
H	-0.89380327	-3.37454058	1.85091367
H	-0.98017390	-3.73946099	4.29218130
H	-0.89254698	2.41421902	0.37656101
H	-0.83414892	4.00746616	2.24002349
H	-0.73454510	4.21830605	4.31415777
H	-0.54147954	3.21157475	6.54152526
H	-0.35152925	1.42598788	7.60623087
H	-0.11244435	-1.01423527	7.60752742

[0]CPPD:	Total	Energy:	-90.8369703512
C	1.22364968	3.85805284	4.06213116
C	-0.05154210	3.27760725	4.24880894
C	2.29722574	3.06414442	3.59290312

C	1.34539807	5.30151468	4.01078571
C	0.19950166	6.09729118	4.20041854
C	-1.19841775	4.06602599	3.99872357
C	2.51491304	5.87587834	3.43629113
C	3.22585560	3.64378613	2.70089023
C	-1.07832862	5.51304634	4.00915455
C	3.33563522	5.08797943	2.62072029
C	-2.35438909	3.47402828	3.43916794
C	3.79164235	2.83664320	1.67936664
C	-2.14806274	6.29658232	3.52612472
C	3.96123628	5.67237090	1.45085147
C	-3.17795264	4.25085280	2.59351817
C	4.17291889	7.07878005	1.29912850
C	-3.10145318	5.69963737	2.66694013
C	3.99701935	3.41488960	0.40964032
C	4.03119632	4.85410495	0.29288518
C	-3.83148445	3.64960721	1.49245814
C	3.90765251	2.62633928	-0.76857191
C	-3.75102025	6.47394275	1.68007208
C	4.19030621	7.66440856	0.05482403
C	3.86790901	5.46045787	-0.98552453
C	-4.07791219	4.42361793	0.33689768
C	3.84446137	6.89164821	-1.10324690
C	-4.07758360	5.87244398	0.44222322
C	3.48088325	3.22188455	-1.96611691
C	3.41494908	4.65309098	-2.06597676
C	-4.02167954	3.82589530	-0.94505376
C	2.89755409	2.44924610	-3.02474404
C	3.29135315	7.48732809	-2.24793540
C	-4.10127295	6.64865043	-0.73842339
C	2.61934910	5.25977926	-3.07970698
C	1.99947302	3.03533342	-3.88591320
C	-3.61422252	4.60841126	-2.04648954
C	2.51385412	6.69908135	-3.13790470
C	-3.68941363	6.05562048	-1.95429477
C	1.74433425	4.44209296	-3.84208307
C	-2.85440638	4.02284009	-3.09084194
C	1.46571173	7.27804719	-3.88296240
C	0.47257374	5.02779799	-4.21761276
C	-3.06188778	6.84280558	-2.94732226
C	-0.68522670	4.24122753	-4.20477502
C	-1.91444222	4.81714334	-3.77474084
C	0.34007587	6.47215223	-4.19641189
C	-2.03486777	6.26075358	-3.72480315
C	-0.94644521	7.05318153	-4.16099169
H	0.29396808	7.19254259	4.14494090

H	-0.14375021	2.18110470	4.22475001
H	2.18970947	1.96879145	3.60341912
H	2.56343267	6.97187459	3.35340454
H	-2.05096154	7.39288505	3.52968429
H	-2.41095034	2.37669525	3.37649094
H	3.70978584	1.74223411	1.76035131
H	-3.68804224	7.57127460	1.73564202
H	-3.82817439	2.55223502	1.40912257
H	3.89508916	1.53016666	-0.67786162
H	3.21909045	8.58362529	-2.30298916
H	-4.09499714	7.74599300	-0.65466367
H	-3.95720910	2.72941127	-1.01626369
H	3.04378537	1.35994748	-3.03735581
H	1.43761376	2.40822992	-4.59253525
H	1.35182827	8.37261639	-3.88207920
H	-3.10822188	7.93945367	-2.86531192
H	-2.74991189	2.92747769	-3.11866406
H	-1.02808523	8.14872300	-4.09232567
H	-0.59342813	3.14524686	-4.18066538
H	4.28281066	7.70620310	2.19496596
H	4.30309896	8.75357020	-0.04104686

S2. Complete citation for references 19, and 54.

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