

Supporting Information for E. Zurek et al.: A Density Functional Study of the ^{13}C NMR Chemical Shifts in Functionalized Single-Walled Carbon Nanotubes

Lattice Parameters and Fractional Coordinates of Pristine and Functionalized SWNTs (PBE functional)

Lattice parameters a, b, c in Angstrom, angles α, β, γ in degrees, energies in Hartree atomic units

(7,0) tube - pristine

$a=13.857201$; $b=13.748613$; $c=8.543734$

$\alpha=89.793671$; $\beta=89.999979$; $\gamma=120.061663$

Energy: -323.9849267 a.u.

k -grid dimension: (1x1x15)

Fractional Coordinates:

C	0.252934	0.383439	0.083709
C	0.354144	0.587375	0.082610
C	0.520261	0.301733	0.084158
C	0.554282	0.714361	0.081938
C	0.326921	0.256444	0.084408
C	0.702537	0.669061	0.082180
C	0.687567	0.485489	0.083156
C	0.718082	0.587418	0.166437
C	0.283514	0.485390	0.166978
C	0.616948	0.383489	0.167527
C	0.416746	0.256393	0.168223
C	0.450822	0.669082	0.166008
C	0.644086	0.714349	0.165772
C	0.268426	0.301726	0.167973
C	0.450864	0.669158	0.332192
C	0.644113	0.714419	0.331966
C	0.616943	0.383519	0.333703
C	0.283531	0.485430	0.333152
C	0.718118	0.587484	0.332610
C	0.268485	0.301778	0.334163
C	0.416769	0.256474	0.334419
C	0.252956	0.383458	0.417531
C	0.687582	0.485525	0.416988
C	0.354173	0.587437	0.416457
C	0.554323	0.714440	0.415801
C	0.702568	0.669136	0.416030
C	0.520250	0.301761	0.417970
C	0.326948	0.256478	0.418216
C	0.252962	0.383422	0.583715

C	0.702591	0.669126	0.582198
C	0.554319	0.714448	0.581953
C	0.326965	0.256481	0.584368
C	0.687561	0.485481	0.583180
C	0.520221	0.301740	0.584134
C	0.354142	0.587402	0.582638
C	0.718122	0.587437	0.666462
C	0.616894	0.383466	0.667558
C	0.416756	0.256459	0.668201
C	0.268507	0.301754	0.667975
C	0.283512	0.485367	0.667019
C	0.644136	0.714426	0.665748
C	0.450829	0.669137	0.666007
C	0.616923	0.383532	0.833729
C	0.268539	0.301829	0.834160
C	0.416795	0.256528	0.834399
C	0.718156	0.587466	0.832641
C	0.450822	0.669186	0.832195
C	0.283533	0.485406	0.833190
C	0.644192	0.714506	0.831945
C	0.554326	0.714481	0.915759
C	0.702625	0.669149	0.916010
C	0.687579	0.485516	0.917010
C	0.326998	0.256555	0.918230
C	0.252993	0.383482	0.917556
C	0.520263	0.301817	0.917992
C	0.354139	0.587418	0.916461

(7,0) tube – NH functionalized at Site I

a=13.867291; b=13.824247; c=8.539359

α =89.822696; β =90.022222; γ =58.864292

Energy: -334.5673525 a.u.

k-grid dimension: (1x1x15)

Fractional Coordinates:

H	0.169465	0.395899	0.501012
C	0.527014	0.276454	0.084583
C	0.665473	0.502279	0.083230
C	0.675007	0.321804	0.084160
C	0.322286	0.395318	0.081670
C	0.496330	0.688215	0.082202
C	0.304208	0.727892	0.081947
C	0.231478	0.600685	0.082819
C	0.423682	0.314157	0.168303
C	0.692680	0.401386	0.167545
C	0.614858	0.278849	0.168380
C	0.595257	0.606002	0.167098

C	0.392460	0.730753	0.165800
C	0.248578	0.680037	0.166121
C	0.253906	0.501053	0.167294
C	0.613370	0.280325	0.334640
C	0.692443	0.401668	0.334025
C	0.253448	0.500449	0.330813
C	0.595369	0.606154	0.332323
C	0.392658	0.730572	0.332228
C	0.249826	0.678564	0.332441
C	0.423001	0.313465	0.331480
C	0.312988	0.388159	0.413307
C	0.673311	0.323273	0.418288
C	0.523660	0.280195	0.417306
C	0.665561	0.502519	0.417344
C	0.305288	0.726413	0.416097
C	0.496542	0.688347	0.416393
C	0.235056	0.597134	0.415656
C	0.523683	0.280145	0.585418
C	0.235117	0.597068	0.583631
C	0.305284	0.726401	0.581957
C	0.496521	0.688353	0.582214
C	0.665572	0.502521	0.583227
C	0.673304	0.323280	0.584163
C	0.313079	0.388068	0.588130
C	0.423062	0.313306	0.670802
C	0.253564	0.500337	0.669430
C	0.249850	0.678530	0.666016
C	0.392643	0.730576	0.665872
C	0.595378	0.606153	0.667158
C	0.692448	0.401672	0.667620
C	0.613355	0.280348	0.668179
C	0.254016	0.500975	0.832918
C	0.248591	0.680030	0.832291
C	0.392447	0.730755	0.832297
C	0.614853	0.278872	0.834450
C	0.595257	0.606008	0.832388
C	0.692694	0.401389	0.834102
C	0.423708	0.314062	0.833975
C	0.322336	0.395261	0.919704
C	0.231531	0.600644	0.916305
C	0.304186	0.727916	0.916081
C	0.496338	0.688209	0.916401
C	0.675000	0.321823	0.918293
C	0.527024	0.276448	0.918171
C	0.665483	0.502278	0.917357
N	0.255264	0.338610	0.501069

(7,0) tube – NH functionalized at Site II

a=13.861787; b=13.819853; c=8.563072

$\alpha=90.014257$; $\beta=91.036877$; $\gamma=59.873191$

Energy: -334.579522 a.u.

k-grid dimension: (1x1x15)

Fractional Coordinates:

H	0.348994	0.233491	0.455944
C	0.532976	0.273286	0.075576
C	0.663153	0.505195	0.085709
C	0.675955	0.323164	0.083839
C	0.330979	0.388769	0.079573
C	0.495848	0.687620	0.083460
C	0.305545	0.724719	0.080746
C	0.237235	0.592988	0.082419
C	0.433393	0.301269	0.153840
C	0.691469	0.404121	0.169184
C	0.618930	0.276635	0.165644
C	0.593143	0.606905	0.169010
C	0.392890	0.729651	0.165863
C	0.252001	0.674901	0.164682
C	0.262985	0.491097	0.165606
C	0.614877	0.278608	0.331899
C	0.689948	0.404756	0.335324
C	0.255023	0.495425	0.333143
C	0.593121	0.607219	0.335058
C	0.392852	0.730016	0.331858
C	0.252376	0.675122	0.330388
C	0.441443	0.274499	0.312176
C	0.294569	0.397939	0.429144
C	0.670206	0.326330	0.417340
C	0.530556	0.265451	0.409883
C	0.662708	0.505139	0.419827
C	0.305704	0.725434	0.414597
C	0.496114	0.687881	0.417614
C	0.235259	0.595454	0.413561
C	0.524581	0.272981	0.577819
C	0.231322	0.599718	0.579812
C	0.304448	0.726986	0.580738
C	0.495751	0.687852	0.583689
C	0.662404	0.505149	0.585750
C	0.670162	0.325966	0.583087
C	0.316951	0.398712	0.588646
C	0.421225	0.314336	0.662913
C	0.258449	0.501371	0.668567
C	0.247206	0.680824	0.663764

C	0.392515	0.730606	0.665931
C	0.592914	0.606890	0.669148
C	0.689544	0.404418	0.669096
C	0.611948	0.280400	0.663101
C	0.261666	0.498714	0.833201
C	0.247825	0.679863	0.830513
C	0.392302	0.730547	0.831912
C	0.615837	0.279577	0.829338
C	0.592806	0.607001	0.835054
C	0.691068	0.404335	0.835321
C	0.425759	0.315133	0.828269
C	0.330003	0.394666	0.914345
C	0.234488	0.597551	0.916352
C	0.304769	0.726459	0.914570
C	0.495853	0.687530	0.917456
C	0.674907	0.323589	0.917148
C	0.530006	0.275397	0.910839
C	0.663186	0.505005	0.919736
N	0.337913	0.288885	0.367822

(8,0) tube – pristine

a=14.304557; b=14.192602; c=8.536917

$\alpha=89.992827$; $\beta=90.103767$; $\gamma=61.541178$

Energy: -370.4135893 a.u.

k-grid dimension: (1x1x11)

Fractional Coordinates:

C	0.419231	0.338333	0.099175
C	0.285975	0.527145	0.098761
C	0.290609	0.696808	0.098750
C	0.430196	0.749055	0.099146
C	0.613115	0.242611	0.099823
C	0.624037	0.653112	0.099707
C	0.757488	0.464397	0.100221
C	0.752807	0.294844	0.100260
C	0.338409	0.427682	0.182864
C	0.269173	0.621550	0.182609
C	0.347151	0.741497	0.182866
C	0.515895	0.273287	0.183432
C	0.527430	0.718113	0.183361
C	0.704807	0.563811	0.183942
C	0.696230	0.250137	0.184007
C	0.774246	0.370061	0.184257
C	0.338391	0.427659	0.348907
C	0.515872	0.273275	0.349480
C	0.269278	0.621400	0.348679
C	0.347331	0.741266	0.348909

C	0.527511	0.718136	0.349393
C	0.696063	0.250229	0.350076
C	0.704783	0.563912	0.349983
C	0.773995	0.370202	0.350300
C	0.419245	0.338372	0.433161
C	0.285875	0.527063	0.432696
C	0.291020	0.696378	0.432684
C	0.613050	0.242508	0.433759
C	0.430394	0.748796	0.433087
C	0.624159	0.653325	0.433729
C	0.752328	0.295193	0.434193
C	0.757188	0.464554	0.434154
C	0.291003	0.696395	0.598727
C	0.430385	0.748809	0.599149
C	0.285872	0.527068	0.598773
C	0.624157	0.653322	0.599742
C	0.757198	0.464549	0.600218
C	0.752343	0.295184	0.600231
C	0.613057	0.242506	0.599835
C	0.419246	0.338374	0.599213
C	0.269261	0.621415	0.682634
C	0.347301	0.741304	0.682817
C	0.527504	0.718139	0.683448
C	0.338390	0.427663	0.682928
C	0.696076	0.250219	0.684019
C	0.704785	0.563909	0.684018
C	0.774024	0.370188	0.684218
C	0.515874	0.273274	0.683505
C	0.269154	0.621563	0.848706
C	0.347122	0.741533	0.848861
C	0.338406	0.427684	0.848970
C	0.515897	0.273287	0.849550
C	0.527423	0.718116	0.849479
C	0.696238	0.250134	0.850090
C	0.774270	0.370050	0.850265
C	0.704808	0.563807	0.850058
C	0.419231	0.338335	0.933190
C	0.285968	0.527151	0.932707
C	0.290596	0.696822	0.932655
C	0.430186	0.749067	0.933084
C	0.613118	0.242610	0.933767
C	0.624032	0.653111	0.933752
C	0.757495	0.464396	0.934154
C	0.752817	0.294840	0.934167

(8,0) tube – NH functionalized at Site I

a=14.342620; b=14.346525; c=8.543940
 $\alpha=89.990726$; $\beta=90.098649$; $\gamma=59.943673$
Energy: -380.9871409 a.u.
k-grid dimension: (1x1x11)

Fractional Coordinates:

H	0.287759	0.301122	0.517076
C	0.416505	0.334032	0.097398
C	0.289586	0.527880	0.099100
C	0.291918	0.697037	0.098571
C	0.428236	0.751034	0.099128
C	0.612892	0.246390	0.100144
C	0.624203	0.653197	0.099998
C	0.759669	0.462766	0.100216
C	0.752569	0.296459	0.100098
C	0.336333	0.427885	0.182862
C	0.273747	0.620690	0.182575
C	0.346548	0.742166	0.182615
C	0.516725	0.270375	0.183455
C	0.526366	0.719858	0.183473
C	0.706664	0.563031	0.184060
C	0.694263	0.254881	0.184033
C	0.774802	0.369718	0.183994
C	0.335769	0.427255	0.346762
C	0.516351	0.269147	0.347084
C	0.275108	0.619516	0.348857
C	0.346792	0.741883	0.349098
C	0.526404	0.719988	0.349404
C	0.692658	0.256252	0.350265
C	0.706724	0.563144	0.349985
C	0.774370	0.369990	0.350517
C	0.409541	0.323653	0.428781
C	0.293127	0.525218	0.431388
C	0.293328	0.695681	0.432788
C	0.609378	0.249579	0.432352
C	0.428342	0.751147	0.433149
C	0.624343	0.653485	0.433536
C	0.750627	0.297976	0.434287
C	0.759629	0.462985	0.434235
C	0.293250	0.695754	0.598597
C	0.428319	0.751151	0.599073
C	0.293115	0.525282	0.600069
C	0.624315	0.653478	0.599933
C	0.759599	0.462996	0.600151
C	0.750677	0.297958	0.600108
C	0.609455	0.249602	0.601212
C	0.409712	0.323774	0.603720

C	0.274959	0.619636	0.682453
C	0.346720	0.741945	0.682613
C	0.526368	0.719970	0.683434
C	0.335915	0.427373	0.685074
C	0.692763	0.256200	0.683818
C	0.706660	0.563145	0.684032
C	0.774367	0.370000	0.684004
C	0.516448	0.269366	0.685980
C	0.273601	0.620810	0.848745
C	0.346477	0.742232	0.849105
C	0.336431	0.427993	0.848950
C	0.516789	0.270554	0.849572
C	0.526339	0.719838	0.849361
C	0.694337	0.254847	0.850076
C	0.774791	0.369729	0.850536
C	0.706601	0.563028	0.849950
C	0.416556	0.334137	0.934943
C	0.289558	0.527948	0.932390
C	0.291845	0.697101	0.932843
C	0.428207	0.751040	0.933091
C	0.612929	0.246422	0.933515
C	0.624169	0.653196	0.933476
C	0.759638	0.462777	0.934178
C	0.752600	0.296449	0.934357
N	0.371103	0.258996	0.516619

(8,0) tube – NH functionalized at Site II

a=14.195645; b=14.219611; c=8.552587

$\alpha=90.060356$; $\beta=89.406171$; $\gamma=63.455044$

Energy: -380.997552 a.u.

k-grid dimension: (1x1x11)

Fractional Coordinates:

H	0.345214	0.892388	0.307046
C	0.418464	0.339309	0.099373
C	0.288825	0.524217	0.099963
C	0.294005	0.691506	0.096380
C	0.431614	0.750648	0.104634
C	0.610233	0.243034	0.098165
C	0.623922	0.647560	0.106252
C	0.756784	0.463397	0.100574
C	0.752767	0.293949	0.097935
C	0.340233	0.427021	0.183695
C	0.272620	0.617752	0.184154
C	0.340219	0.746888	0.177817
C	0.513079	0.274818	0.182716
C	0.529361	0.717375	0.190822

C	0.703425	0.560430	0.186854
C	0.694601	0.249472	0.181820
C	0.774284	0.369488	0.182988
C	0.341682	0.427601	0.349753
C	0.513469	0.274666	0.348705
C	0.275399	0.618875	0.350456
C	0.315727	0.767763	0.336433
C	0.534138	0.721458	0.358790
C	0.694868	0.249396	0.347790
C	0.703997	0.560032	0.352433
C	0.774524	0.369370	0.348880
C	0.419195	0.340119	0.433409
C	0.293512	0.525243	0.433712
C	0.287318	0.701942	0.431847
C	0.610426	0.242773	0.432103
C	0.443258	0.778185	0.455424
C	0.627290	0.647959	0.437860
C	0.752926	0.293697	0.432098
C	0.757432	0.462863	0.434358
C	0.295460	0.699071	0.599330
C	0.440308	0.754653	0.612979
C	0.293449	0.525741	0.599261
C	0.630059	0.646887	0.604153
C	0.759032	0.462464	0.600399
C	0.753090	0.293783	0.597989
C	0.610572	0.242860	0.598161
C	0.419400	0.340405	0.599316
C	0.278084	0.619165	0.681971
C	0.351852	0.745554	0.686458
C	0.537163	0.709423	0.692900
C	0.341851	0.428333	0.683647
C	0.694892	0.249353	0.681871
C	0.708328	0.559561	0.686428
C	0.775619	0.368745	0.682841
C	0.513415	0.275186	0.682845
C	0.276194	0.616835	0.847865
C	0.352675	0.739627	0.851615
C	0.340958	0.427123	0.849688
C	0.513376	0.274948	0.848769
C	0.534765	0.709113	0.857606
C	0.694821	0.249550	0.847867
C	0.775684	0.368779	0.848909
C	0.707172	0.559522	0.852795
C	0.418523	0.339438	0.933309
C	0.289715	0.524440	0.933507
C	0.296789	0.691367	0.931941

C	0.436223	0.745348	0.939245
C	0.610187	0.243160	0.932135
C	0.627273	0.645254	0.940173
C	0.758553	0.462344	0.934541
C	0.753008	0.293693	0.932085
N	0.340918	0.846615	0.397458

(8,0) tube – NH functionalized at Site I, three unit cells

a=14.340345; b=14.328903; c=12.814004

$\alpha=89.986276$; $\beta=90.083224$; $\gamma=60.128934$

Energy: -566.1897921 a.u.

k-grid dimension: (1x1x8)

Fractional Coordinates:

H	0.288039	0.299920	0.499791
C	0.271273	0.622285	0.055061
C	0.337168	0.428858	0.054799
C	0.346365	0.742231	0.055159
C	0.526445	0.719573	0.055294
C	0.517167	0.272046	0.055099
C	0.706390	0.563064	0.055605
C	0.696281	0.252681	0.055803
C	0.774981	0.369512	0.055921
C	0.287807	0.528639	0.110615
C	0.291287	0.697355	0.111087
C	0.428478	0.750620	0.111131
C	0.624236	0.653287	0.111325
C	0.613898	0.244873	0.111179
C	0.759231	0.462943	0.111710
C	0.753023	0.295869	0.111924
C	0.417887	0.336330	0.111492
C	0.417160	0.335155	0.220486
C	0.291763	0.696995	0.221660
C	0.288630	0.528122	0.221696
C	0.428587	0.750658	0.221786
C	0.624298	0.653413	0.222216
C	0.752520	0.296302	0.222502
C	0.613237	0.245547	0.222225
C	0.759197	0.463083	0.222370
C	0.273008	0.620886	0.277619
C	0.346838	0.741768	0.277589
C	0.336703	0.427950	0.277368
C	0.516604	0.270972	0.277651
C	0.526550	0.719753	0.277943
C	0.774316	0.369951	0.278342
C	0.694551	0.254161	0.278403
C	0.706480	0.563245	0.278258

C	0.335917	0.427059	0.386935
C	0.516173	0.269335	0.387025
C	0.274821	0.619375	0.388415
C	0.347243	0.741394	0.388537
C	0.526655	0.719910	0.388597
C	0.706574	0.563422	0.388908
C	0.692590	0.255844	0.389167
C	0.773787	0.370329	0.389309
C	0.409541	0.323463	0.441517
C	0.293120	0.524766	0.443387
C	0.609016	0.249348	0.443871
C	0.293725	0.695132	0.444350
C	0.428815	0.750796	0.444534
C	0.624484	0.653713	0.444692
C	0.759205	0.463388	0.445112
C	0.750041	0.298186	0.445140
C	0.293714	0.695145	0.554948
C	0.428810	0.750797	0.555157
C	0.624479	0.653710	0.555647
C	0.293125	0.524776	0.555999
C	0.750058	0.298175	0.555753
C	0.759208	0.463385	0.555727
C	0.609030	0.249347	0.556626
C	0.409560	0.323479	0.558344
C	0.274802	0.619396	0.610865
C	0.347229	0.741411	0.610906
C	0.526654	0.719902	0.611409
C	0.692624	0.255822	0.611580
C	0.773807	0.370317	0.611621
C	0.706570	0.563412	0.611724
C	0.335950	0.427077	0.612639
C	0.516194	0.269359	0.613184
C	0.272987	0.620914	0.721656
C	0.336733	0.427975	0.722205
C	0.346820	0.741791	0.721855
C	0.526545	0.719747	0.722062
C	0.516625	0.270996	0.722557
C	0.706479	0.563234	0.722373
C	0.694596	0.254128	0.722352
C	0.774354	0.369928	0.722593
C	0.288636	0.528141	0.777677
C	0.291742	0.697022	0.777638
C	0.428581	0.750668	0.777905
C	0.624297	0.653398	0.778117
C	0.613269	0.245544	0.778290
C	0.759215	0.463069	0.778472

C	0.752569	0.296270	0.778410
C	0.417186	0.335176	0.779377
C	0.417900	0.336347	0.888371
C	0.291280	0.697365	0.888213
C	0.287812	0.528649	0.888756
C	0.428474	0.750624	0.888560
C	0.624232	0.653282	0.889008
C	0.753052	0.295848	0.888994
C	0.613914	0.244870	0.889339
C	0.759241	0.462937	0.889133
C	0.271270	0.622291	0.944216
C	0.346365	0.742235	0.944287
C	0.337174	0.428862	0.944769
C	0.517178	0.272050	0.945102
C	0.526447	0.719571	0.944708
C	0.774990	0.369506	0.945022
C	0.696297	0.252673	0.944967
C	0.706391	0.563058	0.945023
N	0.371305	0.258420	0.499916

(8,0) tube – NH functionalized at Site I, four unit cells

a=14.347618; b=14.284294; c=17.082223

$\alpha=89.989590$; $\beta=90.078239$; $\gamma=60.851243$

Energy: -751.3944498 a.u.

k-grid dimension: (1x1x6)

Fractional Coordinates:

H	0.288692	0.297676	0.258094
C	0.417536	0.335721	0.048304
C	0.288875	0.527043	0.049372
C	0.291848	0.696448	0.049603
C	0.429506	0.749660	0.049613
C	0.612223	0.245645	0.049703
C	0.623809	0.652688	0.049721
C	0.758146	0.463783	0.050018
C	0.752038	0.296181	0.050168
C	0.337463	0.427099	0.090985
C	0.273068	0.619873	0.091497
C	0.347634	0.740935	0.091528
C	0.515701	0.271757	0.091168
C	0.527083	0.718592	0.091608
C	0.705342	0.563515	0.091830
C	0.693671	0.253942	0.092015
C	0.773424	0.370520	0.092041
C	0.336445	0.425971	0.173285
C	0.515165	0.269785	0.173325
C	0.274942	0.618130	0.174554

C	0.348303	0.740248	0.174689
C	0.527314	0.718881	0.174634
C	0.691547	0.255616	0.175044
C	0.705493	0.563878	0.174849
C	0.772567	0.371110	0.175213
C	0.409372	0.323100	0.214188
C	0.293418	0.523239	0.215718
C	0.294276	0.693995	0.216506
C	0.607668	0.249373	0.216029
C	0.430061	0.749516	0.216628
C	0.624277	0.653448	0.216707
C	0.748997	0.298386	0.217042
C	0.757792	0.464382	0.217023
C	0.294284	0.693984	0.299414
C	0.430057	0.749512	0.299572
C	0.293416	0.523238	0.300249
C	0.624271	0.653452	0.299934
C	0.757787	0.464385	0.299954
C	0.748995	0.298386	0.299965
C	0.607675	0.249365	0.300684
C	0.409393	0.323103	0.302074
C	0.274951	0.618120	0.341347
C	0.348308	0.740238	0.341338
C	0.527315	0.718882	0.341781
C	0.336454	0.425964	0.342798
C	0.691555	0.255612	0.341851
C	0.705491	0.563876	0.341987
C	0.772564	0.371112	0.341821
C	0.515180	0.269789	0.343182
C	0.273075	0.619858	0.424400
C	0.347636	0.740922	0.424498
C	0.337464	0.427088	0.425102
C	0.515696	0.271748	0.425342
C	0.527079	0.718598	0.424806
C	0.693660	0.253937	0.424888
C	0.773420	0.370520	0.424994
C	0.705336	0.563523	0.425006
C	0.417535	0.335703	0.467980
C	0.288872	0.527029	0.466586
C	0.291856	0.696431	0.466314
C	0.429509	0.749657	0.466585
C	0.612219	0.245636	0.467030
C	0.623810	0.652691	0.466920
C	0.758137	0.463783	0.466957
C	0.752029	0.296181	0.466844
C	0.418605	0.337447	0.549951

C	0.287838	0.527922	0.549857
C	0.290832	0.697306	0.549236
C	0.429113	0.749739	0.549581
C	0.613218	0.244839	0.550277
C	0.623575	0.652290	0.550104
C	0.758385	0.463364	0.549951
C	0.753096	0.295300	0.549767
C	0.338403	0.428840	0.592033
C	0.270413	0.622193	0.591352
C	0.346248	0.742360	0.591327
C	0.516783	0.273591	0.592276
C	0.526611	0.718084	0.591826
C	0.705139	0.562828	0.592030
C	0.696387	0.251740	0.591871
C	0.775186	0.369332	0.591809
C	0.338761	0.429356	0.674700
C	0.517098	0.274193	0.674925
C	0.269761	0.622801	0.674443
C	0.345864	0.742690	0.674444
C	0.526438	0.717920	0.674804
C	0.697088	0.251200	0.674953
C	0.705086	0.562580	0.675006
C	0.775613	0.368989	0.674942
C	0.419731	0.339226	0.716992
C	0.286948	0.528913	0.716401
C	0.289815	0.698338	0.716438
C	0.614268	0.244239	0.716797
C	0.428707	0.749907	0.716598
C	0.623340	0.651868	0.716790
C	0.754304	0.294451	0.716988
C	0.758716	0.462928	0.716983
C	0.289819	0.698337	0.799473
C	0.428705	0.749907	0.799598
C	0.286944	0.528921	0.799554
C	0.623340	0.651870	0.799854
C	0.758718	0.462927	0.799993
C	0.754312	0.294446	0.800029
C	0.614266	0.244244	0.799936
C	0.419729	0.339230	0.799300
C	0.269764	0.622805	0.841449
C	0.345868	0.742694	0.841574
C	0.526444	0.717916	0.841612
C	0.338766	0.429361	0.841391
C	0.697095	0.251204	0.841953
C	0.705094	0.562573	0.841830
C	0.775627	0.368982	0.842097

C	0.517106	0.274200	0.841593
C	0.270413	0.622204	0.924541
C	0.346246	0.742370	0.924692
C	0.338412	0.428853	0.924056
C	0.516789	0.273602	0.924242
C	0.526613	0.718082	0.924590
C	0.696400	0.251735	0.925035
C	0.775210	0.369326	0.925229
C	0.705144	0.562830	0.924805
C	0.418617	0.337461	0.966336
C	0.287846	0.527929	0.966101
C	0.290829	0.697322	0.966679
C	0.429121	0.749741	0.966617
C	0.613229	0.244853	0.966457
C	0.623582	0.652284	0.966536
C	0.758401	0.463361	0.967025
C	0.753118	0.295292	0.967247
N	0.371244	0.257611	0.258120

(8,0) tube – 2NH functional groups

a=14.363914; b=14.659191; c=8.539752

$\alpha=89.988018$; $\beta=90.050842$; $\gamma=58.243456$

Energy: -391.5650025 a.u.

k-grid dimension: (1x1x11)

Fractional Coordinates:

H	0.326427	0.253761	0.500329
H	0.663624	0.773898	0.500438
C	0.624879	0.260348	0.916938
C	0.624850	0.260354	0.083482
C	0.620713	0.263480	0.584367
C	0.620675	0.263496	0.416001
C	0.535714	0.263361	0.330386
C	0.535763	0.263399	0.669827
C	0.536022	0.264466	0.167286
C	0.536050	0.264479	0.832917
C	0.691203	0.289412	0.833446
C	0.689105	0.290951	0.666891
C	0.691153	0.289444	0.167098
C	0.689036	0.290997	0.333632
C	0.429003	0.301992	0.587427
C	0.428957	0.301941	0.412586
C	0.432780	0.314030	0.080961
C	0.432805	0.314033	0.918963
C	0.731042	0.347094	0.917577
C	0.731013	0.347108	0.083042
C	0.727535	0.349560	0.582965

C	0.727496	0.349584	0.417615
C	0.341756	0.400818	0.669246
C	0.341718	0.400786	0.330468
C	0.341887	0.401787	0.167101
C	0.341908	0.401809	0.832597
C	0.734595	0.430171	0.833545
C	0.732553	0.431560	0.666906
C	0.734546	0.430193	0.167036
C	0.732521	0.431585	0.333660
C	0.287444	0.498974	0.583831
C	0.287455	0.498953	0.415688
C	0.283313	0.501533	0.916457
C	0.283306	0.501531	0.083056
C	0.707195	0.525190	0.083540
C	0.707216	0.525174	0.916939
C	0.703082	0.527783	0.416154
C	0.703067	0.527777	0.584296
C	0.255954	0.596547	0.166433
C	0.255936	0.596561	0.832964
C	0.257936	0.595196	0.666328
C	0.257985	0.595168	0.333070
C	0.648718	0.624899	0.832891
C	0.648728	0.624915	0.167411
C	0.648890	0.625931	0.669525
C	0.648926	0.625962	0.330775
C	0.263064	0.677143	0.582366
C	0.263114	0.677113	0.417012
C	0.259577	0.679597	0.916956
C	0.259601	0.679581	0.082419
C	0.557857	0.712654	0.919038
C	0.557850	0.712679	0.081025
C	0.561615	0.724796	0.587450
C	0.561656	0.724821	0.412634
C	0.301592	0.735663	0.666360
C	0.301667	0.735612	0.333093
C	0.299489	0.737214	0.832901
C	0.299542	0.737172	0.166550
C	0.454613	0.762176	0.832735
C	0.454620	0.762218	0.167081
C	0.454913	0.763235	0.669648
C	0.454926	0.763293	0.330175
C	0.369996	0.763102	0.583994
C	0.370030	0.763101	0.415622
C	0.365815	0.766271	0.916534
C	0.365826	0.766270	0.083072
N	0.409301	0.225351	0.500198

N 0.580914 0.801694 0.500128

(8,0) tube – NCH₃ functionalized

a=14.365735; b=14.467057; c=8.545100

$\alpha=89.979135$; $\beta=90.068483$; $\gamma=59.453040$

Energy: -387.9591787 a.u.

k-grid dimension: (1x1x11)

Fractional Coordinates:

H	0.238347	0.266558	0.414029
H	0.204680	0.387780	0.515465
H	0.238788	0.268292	0.622371
C	0.257338	0.299507	0.516997
C	0.754703	0.295955	0.934146
C	0.762438	0.460618	0.933929
C	0.628039	0.651153	0.933335
C	0.616394	0.245247	0.933517
C	0.431528	0.749239	0.933099
C	0.295989	0.695357	0.932984
C	0.294034	0.527389	0.932575
C	0.419633	0.333645	0.935163
C	0.710347	0.560594	0.849710
C	0.776723	0.368560	0.850332
C	0.697176	0.254252	0.849947
C	0.529837	0.718101	0.849267
C	0.520150	0.269174	0.849680
C	0.340016	0.427914	0.849154
C	0.350161	0.740225	0.849195
C	0.278240	0.619513	0.848918
C	0.519576	0.268058	0.686230
C	0.776173	0.368892	0.683761
C	0.710397	0.560729	0.683842
C	0.695358	0.255731	0.683669
C	0.339405	0.427231	0.685203
C	0.529907	0.718241	0.683368
C	0.350543	0.739809	0.682697
C	0.279728	0.618220	0.682693
C	0.412299	0.322999	0.604052
C	0.612577	0.248527	0.601198
C	0.752469	0.297662	0.599958
C	0.762294	0.460878	0.599920
C	0.628219	0.651480	0.599736
C	0.297524	0.524581	0.600342

C	0.431733	0.749263	0.599054
C	0.297804	0.693642	0.598773
C	0.762306	0.460869	0.433993
C	0.752470	0.297656	0.434128
C	0.628220	0.651477	0.433387
C	0.431724	0.749276	0.433151
C	0.612551	0.248533	0.432363
C	0.297790	0.693656	0.432940
C	0.297497	0.524593	0.431554
C	0.412218	0.323000	0.428573
C	0.776197	0.368873	0.350329
C	0.710404	0.560722	0.349732
C	0.695343	0.255733	0.350236
C	0.529904	0.718245	0.349276
C	0.350516	0.739845	0.349184
C	0.279706	0.618238	0.349029
C	0.519536	0.268039	0.346925
C	0.339338	0.427241	0.346985
C	0.776748	0.368542	0.183760
C	0.697173	0.254246	0.183970
C	0.710354	0.560590	0.183865
C	0.529833	0.718107	0.183377
C	0.520131	0.269161	0.183476
C	0.350135	0.740258	0.182682
C	0.278221	0.619527	0.182795
C	0.339978	0.427918	0.183034
C	0.754711	0.295945	0.099957
C	0.762449	0.460611	0.099990
C	0.628039	0.651152	0.099798
C	0.616387	0.245244	0.100082
C	0.431521	0.749250	0.099107
C	0.295977	0.695372	0.098723
C	0.294020	0.527396	0.099310
C	0.419614	0.333640	0.097489
N	0.373716	0.259917	0.516415

(8,0) tube – NCH₂OH functionalized

a=14.389079; b=14.460426; c=8.543914

α =89.898672; β =89.970177; γ =59.341313

Energy: -404.1608288 a.u.

k-grid dimension: (1x1x11)

Fractional Coordinates:

H	0.237740	0.278590	0.628523
H	0.205233	0.380213	0.482503
H	0.287025	0.162990	0.405272
C	0.417225	0.329459	0.088511

C	0.290829	0.523358	0.090220
C	0.293347	0.691111	0.089181
C	0.428579	0.745028	0.089014
C	0.614060	0.241234	0.090699
C	0.625032	0.646584	0.089392
C	0.760082	0.455856	0.089626
C	0.752777	0.291046	0.089979
C	0.337125	0.423704	0.173977
C	0.275285	0.615507	0.173466
C	0.347362	0.735983	0.172841
C	0.517874	0.265435	0.174256
C	0.526831	0.713770	0.173088
C	0.707517	0.555939	0.173386
C	0.695005	0.249763	0.174225
C	0.774878	0.363563	0.173556
C	0.336528	0.423198	0.337904
C	0.517470	0.264429	0.337769
C	0.276685	0.614355	0.339693
C	0.347655	0.735677	0.339370
C	0.526902	0.713893	0.338995
C	0.693372	0.251213	0.340503
C	0.707610	0.556058	0.339293
C	0.774459	0.363845	0.340093
C	0.410358	0.319170	0.419467
C	0.294458	0.520677	0.422387
C	0.294924	0.689634	0.423329
C	0.610387	0.244722	0.422924
C	0.428736	0.745099	0.423071
C	0.625219	0.646885	0.422935
C	0.750819	0.292620	0.424132
C	0.760076	0.456076	0.423602
C	0.294970	0.689606	0.589228
C	0.428768	0.745055	0.588983
C	0.294410	0.520715	0.591124
C	0.625211	0.646911	0.589320
C	0.760047	0.456106	0.589566
C	0.750792	0.292639	0.589996
C	0.610363	0.244744	0.591747
C	0.410429	0.319009	0.595064
C	0.276723	0.614321	0.673329
C	0.347743	0.735571	0.672855
C	0.526905	0.713890	0.673058
C	0.336473	0.423250	0.676260
C	0.693337	0.251237	0.673977
C	0.707596	0.556098	0.673372
C	0.774367	0.363903	0.673597

C	0.517519	0.264466	0.677065
C	0.275322	0.615459	0.839616
C	0.347434	0.735905	0.839377
C	0.337093	0.423747	0.840213
C	0.517900	0.265459	0.840543
C	0.526852	0.713770	0.838954
C	0.694987	0.249802	0.840300
C	0.774777	0.363611	0.840144
C	0.707521	0.555954	0.839295
C	0.417224	0.329446	0.926067
C	0.290807	0.523367	0.923465
C	0.293369	0.691075	0.923389
C	0.428611	0.744994	0.922998
C	0.614092	0.241217	0.924102
C	0.625036	0.646602	0.922889
C	0.760060	0.455858	0.923578
C	0.752747	0.291074	0.924189
C	0.256979	0.293803	0.509286
N	0.372843	0.255318	0.507789
O	0.233814	0.239220	0.393122

(8,0) tube – CH₂NHCH₂ functionalized

a=14.341350; b=14.343229; c=8.543655

α =89.869991; β =89.869785; γ =59.958462

Energy: -394.9727739 a.u.

k-grid dimension: (1x1x11)

Fractional Coordinates:

H	0.375311	0.200253	0.258798
H	0.255580	0.299428	0.353144
H	0.440352	0.113299	0.500384
H	0.256282	0.298994	0.649792
H	0.376723	0.199747	0.742415
C	0.408380	0.336718	0.080801
C	0.627773	0.654294	0.080924
C	0.758759	0.462787	0.080902
C	0.432021	0.752935	0.081020
C	0.288919	0.531308	0.082994
C	0.744896	0.299956	0.081523
C	0.603846	0.251336	0.082900
C	0.295900	0.698342	0.081710
C	0.708812	0.563119	0.164795
C	0.530193	0.721798	0.164859
C	0.769802	0.371305	0.164881
C	0.350843	0.743141	0.165064
C	0.330881	0.431911	0.166766
C	0.508507	0.273446	0.166863

C	0.684998	0.260127	0.166125
C	0.276454	0.622769	0.166293
C	0.708921	0.563316	0.330635
C	0.530335	0.721962	0.330722
C	0.769006	0.371897	0.331472
C	0.351517	0.742459	0.331637
C	0.331897	0.429763	0.330977
C	0.506288	0.273575	0.331101
C	0.681923	0.262924	0.332231
C	0.279505	0.620207	0.332359
C	0.343184	0.246324	0.367150
C	0.395018	0.318762	0.407640
C	0.628060	0.654702	0.414505
C	0.758623	0.463165	0.415006
C	0.432372	0.752900	0.415157
C	0.597885	0.257257	0.414930
C	0.741339	0.302891	0.415686
C	0.295510	0.526325	0.415066
C	0.299119	0.695333	0.415867
C	0.628139	0.654792	0.580912
C	0.758726	0.463197	0.580873
C	0.432400	0.752985	0.580992
C	0.741385	0.302937	0.581527
C	0.299203	0.695326	0.581717
C	0.597902	0.257387	0.583665
C	0.295646	0.526304	0.583792
C	0.395158	0.318797	0.592157
C	0.343799	0.246045	0.634297
C	0.709115	0.563411	0.664830
C	0.530394	0.722160	0.664892
C	0.769149	0.371905	0.665002
C	0.351563	0.742520	0.665191
C	0.681915	0.263074	0.665730
C	0.279732	0.620135	0.665941
C	0.506345	0.273832	0.668114
C	0.332054	0.429780	0.668378
C	0.769938	0.371308	0.831596
C	0.709001	0.563206	0.830687
C	0.530248	0.721987	0.830772
C	0.350881	0.743203	0.831762
C	0.684979	0.260266	0.831824
C	0.276656	0.622712	0.831997
C	0.508543	0.273650	0.832332
C	0.331015	0.431952	0.832572
C	0.744927	0.299998	0.915674
C	0.758856	0.462814	0.914947

C	0.627845	0.654377	0.914448
C	0.295972	0.698339	0.915865
C	0.432046	0.753013	0.915104
C	0.603847	0.251444	0.915758
C	0.289021	0.531307	0.915919
C	0.408434	0.336783	0.918699
N	0.362227	0.176410	0.500838

(9,0) tube – pristine

a=14.914460; b=15.099456; c=8.542026

$\alpha=89.883408$; $\beta=90.122537$; $\gamma=61.634457$

Energy: -416.8200359 a.u.

k-grid dimension: (1x1x21)

Fractional Coordinates:

C	0.332599	0.413388	0.414464
C	0.332573	0.413386	0.580675
C	0.273170	0.505167	0.663866
C	0.273153	0.505186	0.330091
C	0.273174	0.505202	0.830092
C	0.273221	0.505203	0.163870
C	0.332664	0.413436	0.080666
C	0.332666	0.413423	0.914468
C	0.242878	0.597253	0.913424
C	0.242830	0.597283	0.079609
C	0.242811	0.597256	0.579608
C	0.242867	0.597235	0.413423
C	0.413786	0.333237	0.331308
C	0.413779	0.333204	0.665086
C	0.413835	0.333238	0.165086
C	0.413816	0.333239	0.831305
C	0.245274	0.678270	0.829316
C	0.245325	0.678244	0.163122
C	0.245366	0.678200	0.663125
C	0.245295	0.678250	0.329316
C	0.506732	0.274548	0.415701
C	0.506714	0.274577	0.581877
C	0.280007	0.738392	0.913017
C	0.279943	0.738455	0.079237
C	0.506749	0.274588	0.081874
C	0.506756	0.274544	0.915697
C	0.279977	0.738413	0.579238
C	0.280027	0.738372	0.413022
C	0.599911	0.244647	0.666171
C	0.599896	0.244702	0.332359
C	0.599910	0.244666	0.832360
C	0.599942	0.244617	0.166170

C	0.342239	0.771025	0.829381
C	0.342270	0.770983	0.663110
C	0.342275	0.770989	0.163112
C	0.342224	0.771057	0.329383
C	0.681967	0.246901	0.582687
C	0.682009	0.246839	0.416472
C	0.424564	0.772759	0.579701
C	0.424579	0.772719	0.413438
C	0.424623	0.772648	0.913444
C	0.682020	0.246818	0.916470
C	0.681992	0.246873	0.082689
C	0.424600	0.772703	0.079702
C	0.743584	0.280279	0.666560
C	0.743548	0.280318	0.332826
C	0.517697	0.743178	0.663924
C	0.517687	0.743219	0.330179
C	0.517710	0.743199	0.830186
C	0.743520	0.280347	0.832825
C	0.743587	0.280282	0.166560
C	0.517711	0.743174	0.163916
C	0.777848	0.340762	0.582708
C	0.777916	0.340718	0.416456
C	0.610784	0.685232	0.580729
C	0.610794	0.685214	0.414533
C	0.610842	0.685250	0.914526
C	0.777846	0.340782	0.916461
C	0.610830	0.685275	0.080732
C	0.777800	0.340812	0.082706
C	0.780870	0.421465	0.666149
C	0.692279	0.605270	0.665138
C	0.780832	0.421481	0.332390
C	0.692260	0.605282	0.331326
C	0.692307	0.605313	0.831309
C	0.780816	0.421501	0.832399
C	0.692333	0.605293	0.165157
C	0.780874	0.421484	0.166143
C	0.751365	0.513386	0.581889
C	0.751405	0.513374	0.415707
C	0.751466	0.513395	0.915707
C	0.751433	0.513405	0.081900

(9,0) tube – NH functionalized at Site I

a=15.328593; b=15.203109; c=8.545752

$\alpha=90.006473$; $\beta=90.008557$; $\gamma=58.520472$

Energy: -427.3936389 a.u.

k-grid dimension: (1x1x21)

Fractional Coordinates:

H	0.275974	0.291233	0.499771
C	0.305360	0.400781	0.412439
C	0.305354	0.400757	0.587451
C	0.256083	0.502572	0.669502
C	0.256090	0.502594	0.330411
C	0.257104	0.502874	0.833023
C	0.257101	0.502895	0.166893
C	0.315960	0.406432	0.081130
C	0.315953	0.406416	0.918786
C	0.232941	0.594503	0.916690
C	0.232920	0.594524	0.083249
C	0.235842	0.591281	0.584303
C	0.235831	0.591300	0.415640
C	0.402095	0.324675	0.330767
C	0.402086	0.324652	0.669164
C	0.402834	0.325174	0.166939
C	0.402826	0.325149	0.832996
C	0.236462	0.673593	0.833055
C	0.236416	0.673633	0.166915
C	0.237899	0.672003	0.666681
C	0.237867	0.672034	0.333291
C	0.495342	0.274505	0.415755
C	0.495339	0.274496	0.584214
C	0.267152	0.734881	0.917017
C	0.267121	0.734909	0.082995
C	0.497601	0.271257	0.083297
C	0.497597	0.271250	0.916664
C	0.268721	0.733081	0.582990
C	0.268703	0.733100	0.417021
C	0.587959	0.244188	0.666716
C	0.587962	0.244192	0.333285
C	0.589077	0.242659	0.833131
C	0.589084	0.242653	0.166869
C	0.325658	0.768234	0.833311
C	0.325969	0.767773	0.666813
C	0.325625	0.768267	0.166744
C	0.325943	0.767804	0.333245
C	0.669721	0.242793	0.583013
C	0.669725	0.242790	0.417029
C	0.405137	0.770922	0.583130
C	0.405128	0.770933	0.416970
C	0.404983	0.771106	0.916924
C	0.670969	0.241155	0.917021
C	0.670983	0.241136	0.083023
C	0.404970	0.771108	0.083172

C	0.731799	0.271581	0.666842
C	0.731815	0.271562	0.333240
C	0.497474	0.741169	0.667087
C	0.497468	0.741168	0.333051
C	0.497481	0.741240	0.833121
C	0.732182	0.271193	0.833309
C	0.732207	0.271164	0.166772
C	0.497469	0.741228	0.167017
C	0.766311	0.329337	0.583135
C	0.766321	0.329329	0.416985
C	0.591467	0.680793	0.583184
C	0.591462	0.680786	0.416982
C	0.591557	0.680918	0.916988
C	0.766539	0.329110	0.916941
C	0.591547	0.680906	0.083180
C	0.766550	0.329095	0.083178
C	0.768401	0.409822	0.667092
C	0.674705	0.597848	0.667008
C	0.768410	0.409813	0.333062
C	0.674693	0.597837	0.333169
C	0.674834	0.597901	0.833258
C	0.768531	0.409777	0.833136
C	0.674815	0.597884	0.166922
C	0.768537	0.409763	0.167017
C	0.736400	0.503419	0.583183
C	0.736397	0.503415	0.416990
C	0.736646	0.503415	0.916996
C	0.736638	0.503405	0.083177
N	0.240067	0.370784	0.499874

(9,0) tube – NH functionalized at Site II

a=15.295827; b=15.488841; c=8.556963

$\alpha=90.633749$; $\beta=90.022102$; $\gamma=58.473985$

Energy: -427.4004045 a.u.

k-grid dimension: (1x1x51)

Fractional Coordinates:

H	0.264005	0.328319	0.709111
C	0.308956	0.416955	0.403922
C	0.283440	0.420389	0.561489
C	0.252305	0.507612	0.657917
C	0.261620	0.509967	0.324048
C	0.260395	0.503222	0.826101
C	0.263904	0.508057	0.159109
C	0.321276	0.413567	0.077515
C	0.320041	0.409412	0.911932
C	0.235427	0.594836	0.910427

C	0.234631	0.597819	0.076678
C	0.232641	0.597615	0.578727
C	0.231240	0.599958	0.412410
C	0.397747	0.330702	0.330409
C	0.408555	0.296375	0.679892
C	0.402474	0.332050	0.165021
C	0.406242	0.320527	0.838331
C	0.236981	0.674571	0.829867
C	0.234305	0.677948	0.163731
C	0.237125	0.674955	0.664040
C	0.233464	0.678800	0.330305
C	0.492536	0.271434	0.416845
C	0.496962	0.263780	0.584542
C	0.267345	0.734742	0.915878
C	0.266411	0.736549	0.082257
C	0.498172	0.273857	0.084493
C	0.500280	0.271361	0.919722
C	0.267393	0.735282	0.582409
C	0.265984	0.736949	0.416086
C	0.588308	0.243399	0.665720
C	0.585801	0.245662	0.334210
C	0.591291	0.241052	0.832156
C	0.589254	0.244214	0.168124
C	0.325845	0.767742	0.833858
C	0.325822	0.767945	0.667786
C	0.324887	0.769345	0.167707
C	0.324926	0.769429	0.333921
C	0.667424	0.246466	0.582263
C	0.666927	0.246370	0.416483
C	0.405971	0.769801	0.584913
C	0.405673	0.770022	0.418780
C	0.405865	0.769562	0.918843
C	0.671802	0.242138	0.915935
C	0.670864	0.242995	0.082571
C	0.405810	0.769904	0.084947
C	0.729395	0.275288	0.665769
C	0.728563	0.275473	0.332252
C	0.498853	0.738512	0.669163
C	0.498799	0.738503	0.335387
C	0.498923	0.738359	0.835410
C	0.731194	0.273745	0.832100
C	0.730519	0.274370	0.165920
C	0.498694	0.738506	0.169155
C	0.763139	0.332439	0.582243
C	0.762778	0.332558	0.416140
C	0.592946	0.677898	0.585144

C	0.592727	0.677956	0.419044
C	0.592824	0.677846	0.919080
C	0.764660	0.331490	0.916100
C	0.592814	0.677754	0.085151
C	0.764445	0.331519	0.082328
C	0.766194	0.410959	0.666755
C	0.675561	0.595566	0.668434
C	0.765811	0.410907	0.332815
C	0.675427	0.595424	0.334497
C	0.675629	0.595374	0.834538
C	0.766395	0.410651	0.832907
C	0.675338	0.595441	0.168422
C	0.766125	0.410845	0.166705
C	0.735774	0.502418	0.583758
C	0.735559	0.502497	0.417501
C	0.735728	0.502368	0.917507
C	0.735682	0.502276	0.083743
N	0.311329	0.322816	0.618999

(9,0) tube – NH functionalized at Site I, three unit cells

a=15.069773; b=15.096945; c=12.813582

$\alpha=90.002912$; $\beta=90.004299$; $\gamma=60.150037$

Energy: -635.7998258 a.u.

k-grid dimension: (1x1x16)

Fractional Coordinates:

H	0.285036	0.294140	0.499926
C	0.413869	0.330883	0.054973
C	0.270484	0.506083	0.054959
C	0.248695	0.677813	0.055439
C	0.515959	0.746197	0.055366
C	0.783289	0.419152	0.055376
C	0.600695	0.247261	0.055454
C	0.692360	0.605522	0.055457
C	0.744420	0.280042	0.055484
C	0.342502	0.771729	0.055481
C	0.508065	0.275633	0.110940
C	0.244546	0.597843	0.110912
C	0.423054	0.775137	0.111300
C	0.779835	0.338672	0.111313
C	0.609805	0.687134	0.111311
C	0.752854	0.512118	0.111325
C	0.282587	0.737795	0.111397
C	0.682274	0.248840	0.111391
C	0.329016	0.411413	0.111542
C	0.327829	0.410823	0.220511
C	0.283147	0.737219	0.222119

C	0.681863	0.249441	0.222123
C	0.752870	0.512135	0.222105
C	0.609839	0.687152	0.222098
C	0.779792	0.338756	0.222109
C	0.423139	0.775079	0.222092
C	0.245366	0.597173	0.221921
C	0.507614	0.276517	0.221969
C	0.342971	0.771108	0.277917
C	0.743942	0.280570	0.277935
C	0.599418	0.249263	0.277957
C	0.692442	0.605569	0.277966
C	0.250521	0.676009	0.277974
C	0.269554	0.505588	0.277539
C	0.412906	0.330558	0.277556
C	0.783307	0.419211	0.278035
C	0.516045	0.746221	0.278019
C	0.267909	0.505288	0.386848
C	0.411970	0.329815	0.387053
C	0.516093	0.746299	0.388673
C	0.783397	0.419211	0.388691
C	0.692539	0.605615	0.388750
C	0.743660	0.280808	0.388847
C	0.343178	0.770753	0.388850
C	0.252073	0.674303	0.388818
C	0.598202	0.250927	0.388821
C	0.315740	0.404359	0.441517
C	0.248675	0.593497	0.443700
C	0.504965	0.280400	0.443781
C	0.609972	0.687301	0.444638
C	0.423244	0.775078	0.444674
C	0.753062	0.512169	0.444647
C	0.779823	0.338808	0.444677
C	0.680566	0.250989	0.444681
C	0.284624	0.735401	0.444673
C	0.284620	0.735403	0.555342
C	0.680563	0.250990	0.555340
C	0.779824	0.338805	0.555372
C	0.423239	0.775082	0.555364
C	0.753055	0.512166	0.555410
C	0.609966	0.687296	0.555415
C	0.504956	0.280400	0.556212
C	0.248666	0.593494	0.556290
C	0.315726	0.404350	0.558450
C	0.252063	0.674308	0.611183
C	0.598201	0.250924	0.611187
C	0.343173	0.770760	0.611174

C	0.743662	0.280804	0.611189
C	0.692522	0.605606	0.611311
C	0.516091	0.746289	0.611374
C	0.783388	0.419211	0.611365
C	0.411958	0.329805	0.612924
C	0.267890	0.505282	0.613127
C	0.412903	0.330551	0.722420
C	0.269544	0.505584	0.722437
C	0.250506	0.676016	0.722026
C	0.516048	0.746206	0.722028
C	0.783293	0.419217	0.722022
C	0.599420	0.249254	0.722051
C	0.692434	0.605565	0.722098
C	0.743940	0.280568	0.722100
C	0.342968	0.771110	0.722107
C	0.507615	0.276512	0.778020
C	0.245369	0.597170	0.778063
C	0.423146	0.775071	0.777948
C	0.779783	0.338762	0.777942
C	0.752873	0.512139	0.777961
C	0.609845	0.687154	0.777962
C	0.283155	0.737212	0.777890
C	0.681863	0.249441	0.777897
C	0.327829	0.410820	0.779467
C	0.329019	0.411405	0.888433
C	0.282623	0.737766	0.888609
C	0.682266	0.248859	0.888627
C	0.752875	0.512124	0.888741
C	0.609822	0.687154	0.888751
C	0.423065	0.775142	0.888740
C	0.779839	0.338680	0.888737
C	0.244575	0.597824	0.889069
C	0.508063	0.275635	0.889049
C	0.342521	0.771720	0.944541
C	0.744418	0.280053	0.944552
C	0.600695	0.247271	0.944552
C	0.692376	0.605531	0.944612
C	0.270495	0.506077	0.945016
C	0.248725	0.677796	0.944555
C	0.413871	0.330878	0.945005
C	0.783300	0.419154	0.944683
C	0.515968	0.746210	0.944686
N	0.249611	0.373064	0.499950

(9,0) tube – 2NH functional groups
a=15.223503; b=15.410143; c=8.546682

$\alpha=90.145867$; $\beta=90.008272$; $\gamma=57.561604$

Energy: -437.969197 a.u.

k -grid dimension: (1x1x21)

Fractional Coordinates:

H	0.280840	0.301154	0.496657
H	0.728736	0.728955	0.499253
C	0.313069	0.406949	0.409868
C	0.313026	0.406918	0.584857
C	0.265270	0.508231	0.667435
C	0.265318	0.508277	0.328191
C	0.266625	0.508496	0.830651
C	0.266661	0.508531	0.164997
C	0.324186	0.412085	0.078531
C	0.324149	0.412053	0.916334
C	0.246451	0.598009	0.915018
C	0.246410	0.598072	0.081455
C	0.249129	0.594774	0.582356
C	0.249135	0.594816	0.414086
C	0.411108	0.329045	0.327903
C	0.411076	0.328935	0.666216
C	0.411887	0.329655	0.163973
C	0.411838	0.329559	0.830195
C	0.254643	0.673219	0.831777
C	0.254498	0.673348	0.165427
C	0.256399	0.671390	0.665142
C	0.256316	0.671475	0.332046
C	0.505854	0.277374	0.412541
C	0.505861	0.277299	0.581148
C	0.288445	0.730809	0.915950
C	0.288334	0.730921	0.081792
C	0.508145	0.274545	0.080209
C	0.508131	0.274457	0.913455
C	0.291565	0.727688	0.581726
C	0.291495	0.727754	0.416038
C	0.599832	0.246568	0.663508
C	0.599795	0.246658	0.329921
C	0.600920	0.245323	0.829737
C	0.600916	0.245408	0.163696
C	0.348652	0.761971	0.832174
C	0.350483	0.760213	0.665610
C	0.348513	0.762120	0.165877
C	0.350361	0.760341	0.332486
C	0.681089	0.247230	0.579719
C	0.681094	0.247236	0.413762
C	0.429270	0.765245	0.583278
C	0.429225	0.765305	0.414939

C	0.426032	0.767979	0.915826
C	0.682400	0.245807	0.913717
C	0.682440	0.245797	0.079768
C	0.425962	0.768057	0.082275
C	0.740691	0.278660	0.663504
C	0.740702	0.278655	0.330310
C	0.517409	0.747783	0.668638
C	0.517384	0.747793	0.329381
C	0.517158	0.746574	0.831861
C	0.741421	0.277975	0.830322
C	0.741485	0.277927	0.163468
C	0.517106	0.746572	0.166106
C	0.773132	0.336999	0.580178
C	0.773147	0.336978	0.414235
C	0.620048	0.699445	0.586256
C	0.620059	0.699425	0.411336
C	0.614799	0.688792	0.917655
C	0.774815	0.335583	0.914103
C	0.614746	0.688761	0.079847
C	0.774795	0.335582	0.080202
C	0.775649	0.416234	0.664267
C	0.697614	0.601951	0.667499
C	0.775616	0.416225	0.330814
C	0.697521	0.601896	0.329225
C	0.697220	0.601181	0.831413
C	0.777153	0.415056	0.830521
C	0.697114	0.601139	0.165310
C	0.777124	0.415039	0.164513
C	0.747281	0.508303	0.582222
C	0.747244	0.508281	0.413694
C	0.750571	0.505905	0.914498
C	0.750595	0.505872	0.081311
N	0.245357	0.380256	0.497102
N	0.648557	0.765116	0.499122

(9,0) tube – NCH₃ functionalized

a=15.387060; b=15.350960; c=8.546004

α =89.931933; β =89.981931; γ =59.473497

Energy: -434.3654055 a.u.

k-grid dimension: (1x1x21)

Fractional Coordinates:

H	0.240380	0.256422	0.582923
H	0.270622	0.248663	0.380260
H	0.367202	0.214535	0.523890
C	0.286958	0.267348	0.496586
C	0.322159	0.403911	0.410627

C	0.321924	0.403946	0.586135
C	0.274586	0.503932	0.667860
C	0.274766	0.503901	0.328487
C	0.275884	0.504255	0.831345
C	0.275994	0.504242	0.165021
C	0.333198	0.409759	0.079511
C	0.333137	0.409766	0.917187
C	0.252562	0.594361	0.914739
C	0.252591	0.594357	0.081247
C	0.255063	0.591269	0.582344
C	0.255101	0.591272	0.413652
C	0.417620	0.329799	0.329310
C	0.417516	0.329911	0.667585
C	0.418337	0.330359	0.165430
C	0.418294	0.330432	0.831468
C	0.256044	0.672719	0.830876
C	0.256049	0.672736	0.164756
C	0.257378	0.671153	0.664483
C	0.257381	0.671170	0.331155
C	0.509503	0.281022	0.414256
C	0.509438	0.281160	0.582742
C	0.286470	0.733887	0.914667
C	0.286461	0.733904	0.080656
C	0.511695	0.277977	0.081810
C	0.511665	0.278038	0.915165
C	0.288020	0.732062	0.580614
C	0.288010	0.732080	0.414718
C	0.600967	0.252498	0.665213
C	0.601020	0.252371	0.331783
C	0.602020	0.251034	0.831577
C	0.602068	0.250926	0.165391
C	0.344202	0.768008	0.830792
C	0.344519	0.767512	0.664301
C	0.344190	0.768035	0.164303
C	0.344514	0.767529	0.330803
C	0.681315	0.253220	0.581395
C	0.681331	0.253183	0.415466
C	0.422605	0.772256	0.580574
C	0.422604	0.772256	0.414408
C	0.422408	0.772421	0.914345
C	0.682566	0.251578	0.915457
C	0.682578	0.251548	0.081429
C	0.422404	0.772430	0.080632
C	0.742093	0.283476	0.665130
C	0.742096	0.283461	0.331539
C	0.513762	0.744430	0.664504

C	0.513760	0.744423	0.330478
C	0.513695	0.744395	0.830505
C	0.742433	0.283103	0.831577
C	0.742448	0.283077	0.165087
C	0.513691	0.744395	0.164473
C	0.776144	0.341352	0.581275
C	0.776133	0.341353	0.415097
C	0.606489	0.686178	0.580643
C	0.606488	0.686175	0.414476
C	0.606367	0.686070	0.914471
C	0.776250	0.341136	0.915066
C	0.606363	0.686068	0.080643
C	0.776246	0.341130	0.081319
C	0.778784	0.420796	0.665003
C	0.688241	0.605205	0.664571
C	0.778766	0.420796	0.331029
C	0.688233	0.605203	0.330788
C	0.688175	0.605163	0.830807
C	0.778747	0.420736	0.831051
C	0.688170	0.605158	0.164554
C	0.778740	0.420734	0.164983
C	0.748334	0.512678	0.580934
C	0.748330	0.512676	0.414749
C	0.748208	0.512606	0.914750
C	0.748203	0.512602	0.080929
N	0.257084	0.374513	0.497844

(9,0) tube – NCH₂OH functionalized

a=15.470916; b=15.163466; c=8.545064

α =89.947564; β =89.971135; γ =58.272002

Energy: -450.5616086 a.u.

k-grid dimension: (1x1x21)

Fractional Coordinates:

H	0.278197	0.238525	0.365567
H	0.361872	0.204181	0.531023
H	0.247804	0.167424	0.606442
C	0.282525	0.255623	0.490066
C	0.309220	0.398423	0.412617
C	0.309247	0.398017	0.588321
C	0.257995	0.500745	0.669926
C	0.258251	0.501021	0.330489
C	0.259383	0.501283	0.833326
C	0.259563	0.501392	0.167169
C	0.320002	0.404750	0.081476
C	0.319908	0.404681	0.919255
C	0.233979	0.593709	0.916815

C	0.233988	0.593776	0.083319
C	0.236701	0.590318	0.584435
C	0.236729	0.590483	0.415823
C	0.406631	0.323759	0.331217
C	0.406485	0.323533	0.669574
C	0.407253	0.324418	0.167336
C	0.407130	0.324278	0.833511
C	0.236806	0.673311	0.832953
C	0.236751	0.673418	0.166934
C	0.238237	0.671587	0.666597
C	0.238158	0.671774	0.333308
C	0.499086	0.274032	0.416143
C	0.499028	0.274015	0.584700
C	0.267465	0.734429	0.916809
C	0.267427	0.734495	0.082798
C	0.501297	0.270979	0.083720
C	0.501234	0.270988	0.917072
C	0.269034	0.732535	0.582773
C	0.268982	0.732652	0.416856
C	0.590940	0.243803	0.667088
C	0.590999	0.243726	0.333628
C	0.591970	0.242354	0.833420
C	0.592046	0.242262	0.167290
C	0.325685	0.767388	0.832951
C	0.325998	0.766914	0.666442
C	0.325635	0.767483	0.166420
C	0.325945	0.767031	0.332944
C	0.671790	0.242608	0.583249
C	0.671844	0.242546	0.417294
C	0.404386	0.770199	0.582709
C	0.404381	0.770228	0.416480
C	0.404220	0.770305	0.916437
C	0.673014	0.240983	0.917281
C	0.673056	0.240933	0.083273
C	0.404208	0.770326	0.082770
C	0.733126	0.271524	0.666910
C	0.733176	0.271461	0.333403
C	0.495866	0.741066	0.666535
C	0.495859	0.741068	0.332574
C	0.495796	0.741010	0.832593
C	0.733432	0.271176	0.833381
C	0.733487	0.271116	0.166934
C	0.495788	0.741010	0.166526
C	0.767276	0.329388	0.583092
C	0.767284	0.329370	0.416941
C	0.589537	0.681742	0.582655

C	0.589531	0.681740	0.416471
C	0.589393	0.681601	0.916474
C	0.767268	0.329248	0.916891
C	0.589379	0.681598	0.082658
C	0.767267	0.329233	0.083140
C	0.768779	0.410382	0.666866
C	0.673297	0.599294	0.666507
C	0.768759	0.410377	0.332877
C	0.673281	0.599289	0.332744
C	0.673208	0.599241	0.832724
C	0.768688	0.410345	0.832851
C	0.673192	0.599234	0.166524
C	0.768671	0.410343	0.166881
C	0.736063	0.504597	0.582803
C	0.736050	0.504598	0.416665
C	0.735851	0.504542	0.916661
C	0.735838	0.504542	0.082798
N	0.247642	0.365421	0.498820
O	0.214901	0.241100	0.583482

(9,0) tube – CH₂NHCH₂ functionalized

a=15.430757; b=15.203248; c=8.545604

α =90.099092; β =89.954793; γ =57.562416

Energy: -441.3725726 a.u.

k-grid dimension: (1x1x21)

Fractional Coordinates:

H	0.178038	0.272306	0.500057
H	0.238184	0.316606	0.256306
H	0.135896	0.430242	0.352166
H	0.234893	0.320120	0.743699
H	0.134808	0.432650	0.643772
C	0.287615	0.401771	0.406956
C	0.287549	0.401924	0.592023
C	0.248936	0.507766	0.668784
C	0.248626	0.507792	0.330961
C	0.249051	0.509480	0.832869
C	0.248867	0.509534	0.166900
C	0.307081	0.412006	0.080485
C	0.307112	0.411947	0.918535
C	0.226195	0.600858	0.916737
C	0.226102	0.600900	0.083708
C	0.231233	0.595493	0.584542
C	0.231126	0.595493	0.415813
C	0.393336	0.331552	0.330581
C	0.393233	0.331309	0.667738
C	0.395532	0.331089	0.166504

C	0.395502	0.330888	0.831802
C	0.229022	0.680205	0.833349
C	0.228916	0.680254	0.167609
C	0.231657	0.677336	0.667160
C	0.231571	0.677353	0.333775
C	0.486099	0.285678	0.414600
C	0.486054	0.285628	0.583236
C	0.257434	0.742880	0.917609
C	0.257403	0.742897	0.083689
C	0.490370	0.279640	0.082413
C	0.490367	0.279570	0.915323
C	0.260298	0.739593	0.583602
C	0.260282	0.739579	0.417660
C	0.578728	0.255879	0.665372
C	0.578797	0.255828	0.332013
C	0.581122	0.252615	0.831550
C	0.581145	0.252604	0.165808
C	0.313905	0.777728	0.834001
C	0.314507	0.776847	0.667439
C	0.313898	0.777727	0.167360
C	0.314507	0.776829	0.333917
C	0.659694	0.254886	0.581551
C	0.659740	0.254844	0.415600
C	0.391985	0.782017	0.583611
C	0.391999	0.782004	0.417522
C	0.391645	0.782471	0.917479
C	0.662402	0.251393	0.915529
C	0.662427	0.251375	0.081617
C	0.391644	0.782462	0.083689
C	0.721912	0.282423	0.665326
C	0.721964	0.282385	0.331830
C	0.483932	0.753327	0.667343
C	0.483955	0.753309	0.333338
C	0.483830	0.753382	0.833375
C	0.722680	0.281625	0.831904
C	0.722730	0.281591	0.165232
C	0.483848	0.753354	0.167307
C	0.756838	0.339247	0.581747
C	0.756879	0.339226	0.415630
C	0.578588	0.693107	0.583100
C	0.578618	0.693105	0.416895
C	0.578468	0.693109	0.916894
C	0.757179	0.338830	0.915568
C	0.578480	0.693095	0.083117
C	0.757219	0.338809	0.081777
C	0.758994	0.419683	0.665941

C	0.663140	0.609550	0.666540
C	0.759101	0.419642	0.331886
C	0.663207	0.609564	0.332693
C	0.663075	0.609550	0.832749
C	0.758948	0.419612	0.831938
C	0.663129	0.609542	0.166483
C	0.759046	0.419573	0.165872
C	0.726325	0.514089	0.582311
C	0.726383	0.514082	0.416123
C	0.726147	0.514043	0.916156
C	0.726190	0.514028	0.082341
C	0.215611	0.361724	0.365513
C	0.214412	0.363361	0.633164
N	0.227904	0.297413	0.499974

(10,0) tube – pristine

a=15.959352; b=15.958216; c=8.547545

$\alpha=90.000035$; $\beta=90.027009$; $\gamma=120.014285$

Energy: -463.2291762 a.u.

k-grid dimension: (1x1x14)

Fractional Coordinates

C	0.786516	0.594836	0.083388
C	0.768004	0.738046	0.083379
C	0.649506	0.792728	0.083301
C	0.476383	0.738054	0.083194
C	0.314627	0.594829	0.083092
C	0.226107	0.417782	0.083036
C	0.244618	0.274577	0.083050
C	0.363105	0.219885	0.083121
C	0.536229	0.274559	0.083231
C	0.697990	0.417783	0.083333
C	0.754420	0.506310	0.833357
C	0.754417	0.506310	0.666933
C	0.786506	0.594833	0.916964
C	0.791192	0.674679	0.833377
C	0.791186	0.674676	0.666959
C	0.767995	0.738038	0.916950
C	0.719180	0.778725	0.833339
C	0.719179	0.778723	0.666905
C	0.649505	0.792722	0.916879
C	0.565877	0.778719	0.833233
C	0.565880	0.778723	0.666819
C	0.476384	0.738056	0.916769
C	0.389807	0.674678	0.833127
C	0.389804	0.674686	0.666706
C	0.314623	0.594832	0.916667

C	0.258201	0.506304	0.833046
C	0.258188	0.506304	0.666622
C	0.226097	0.417779	0.916612
C	0.221433	0.337943	0.833020
C	0.221416	0.337933	0.666602
C	0.244609	0.274569	0.916621
C	0.293435	0.233890	0.833073
C	0.293425	0.233876	0.666639
C	0.363104	0.219879	0.916699
C	0.446730	0.233889	0.833159
C	0.446730	0.233882	0.666745
C	0.536230	0.274561	0.916806
C	0.622807	0.337933	0.833273
C	0.622808	0.337933	0.666851
C	0.697986	0.417786	0.916908
C	0.754425	0.506310	0.333378
C	0.754412	0.506310	0.166954
C	0.786527	0.594839	0.583380
C	0.786517	0.594836	0.416971
C	0.791197	0.674682	0.333398
C	0.791181	0.674672	0.166980
C	0.768014	0.738055	0.583371
C	0.768005	0.738046	0.416957
C	0.719185	0.778731	0.333361
C	0.719175	0.778717	0.166927
C	0.649511	0.792739	0.583294
C	0.649510	0.792733	0.416886
C	0.565879	0.778725	0.333255
C	0.565879	0.778718	0.166841
C	0.476382	0.738063	0.583187
C	0.476383	0.738065	0.416776
C	0.389805	0.674682	0.333149
C	0.389806	0.674682	0.166727
C	0.314620	0.594833	0.583085
C	0.314616	0.594836	0.416675
C	0.258196	0.506304	0.333067
C	0.258193	0.506304	0.166643
C	0.226096	0.417779	0.583029
C	0.226086	0.417776	0.416620
C	0.221427	0.337939	0.333041
C	0.221422	0.337936	0.166623
C	0.244608	0.274568	0.583043
C	0.244599	0.274559	0.416629
C	0.293431	0.233884	0.333095
C	0.293430	0.233882	0.166661
C	0.363099	0.219874	0.583114

C	0.363098	0.219868	0.416706
C	0.446729	0.233884	0.333181
C	0.446732	0.233888	0.166767
C	0.536230	0.274549	0.583224
C	0.536231	0.274551	0.416813
C	0.622809	0.337929	0.333294
C	0.622806	0.337937	0.166873
C	0.697997	0.417779	0.583325
C	0.697993	0.417782	0.416915

(10,0) tube – NH functionalized at Site I

a=16.263339; b=16.472492; c=8.547996

$\alpha=89.962123$; $\beta=89.976509$; $\gamma=58.317991$

Energy: -473.7927283 a.u.

k-grid dimension: (1x1x15)

Fractional Coordinates

H	0.629458	0.764798	0.500001
C	0.457499	0.728442	0.083498
C	0.634730	0.632478	0.081484
C	0.235241	0.629124	0.083606
C	0.307325	0.727498	0.083365
C	0.758467	0.461862	0.083575
C	0.269402	0.465672	0.083905
C	0.792658	0.298251	0.083488
C	0.725471	0.195573	0.083814
C	0.400004	0.298075	0.083893
C	0.575858	0.194022	0.084012
C	0.545980	0.693648	0.166955
C	0.376240	0.740119	0.167184
C	0.259379	0.688917	0.167016
C	0.238370	0.552251	0.167487
C	0.708455	0.550035	0.167083
C	0.787286	0.376306	0.167311
C	0.771073	0.236548	0.167203
C	0.324967	0.377999	0.167583
C	0.658239	0.180615	0.167680
C	0.486703	0.234414	0.167681
C	0.377410	0.738875	0.333492
C	0.709741	0.550609	0.330780
C	0.259780	0.688535	0.333693
C	0.238167	0.552249	0.333619
C	0.786032	0.377315	0.333621
C	0.770700	0.236915	0.333900
C	0.324834	0.377926	0.333922
C	0.658268	0.180504	0.333808
C	0.486694	0.234329	0.334007

C	0.546315	0.694532	0.330992
C	0.641431	0.641866	0.412437
C	0.459923	0.725894	0.415906
C	0.756250	0.464018	0.415899
C	0.308800	0.725899	0.417214
C	0.235157	0.629037	0.417309
C	0.791066	0.299473	0.417394
C	0.269011	0.465631	0.417415
C	0.725353	0.195630	0.417507
C	0.575881	0.193823	0.417595
C	0.399914	0.297956	0.417707
C	0.459921	0.725892	0.584491
C	0.641422	0.641869	0.587873
C	0.756246	0.464021	0.584696
C	0.791063	0.299474	0.583504
C	0.308803	0.725901	0.583310
C	0.575880	0.193821	0.583986
C	0.399915	0.297951	0.583874
C	0.725349	0.195632	0.583784
C	0.269018	0.465626	0.583878
C	0.235170	0.629027	0.583593
C	0.546311	0.694524	0.669339
C	0.486693	0.234325	0.667606
C	0.786031	0.377314	0.667090
C	0.709735	0.550610	0.669679
C	0.658267	0.180504	0.667636
C	0.324830	0.377922	0.667525
C	0.770689	0.236926	0.667204
C	0.238194	0.552237	0.667510
C	0.377399	0.738882	0.666989
C	0.259794	0.688528	0.667008
C	0.708452	0.550030	0.833349
C	0.486703	0.234406	0.833927
C	0.658233	0.180620	0.833791
C	0.787285	0.376309	0.833403
C	0.324969	0.377995	0.833900
C	0.376231	0.740126	0.833292
C	0.771066	0.236553	0.833898
C	0.238396	0.552235	0.833675
C	0.259392	0.688912	0.833692
C	0.545982	0.693637	0.833384
C	0.634730	0.632474	0.918833
C	0.758467	0.461858	0.917008
C	0.575857	0.194020	0.917581
C	0.400003	0.298069	0.917698
C	0.792655	0.298253	0.917412

C	0.725468	0.195578	0.917489
C	0.307325	0.727496	0.917232
C	0.269413	0.465667	0.917483
C	0.235251	0.629120	0.917306
C	0.457498	0.728441	0.916838
N	0.681157	0.692610	0.500096

(10,0) tube – NH functionalized at Site II

a=16.284159; b=16.649963; c=8.557934

$\alpha=89.536000$; $\beta=90.156566$; $\gamma=58.208194$

Energy: -473.8041794 a.u.

k-grid dimension: (1x1x15)

Fractional Coordinates

H	0.651246	0.732066	0.711370
C	0.456828	0.726453	0.084820
C	0.631965	0.626956	0.078250
C	0.236780	0.627135	0.082464
C	0.308657	0.724544	0.083003
C	0.757372	0.459161	0.077218
C	0.269652	0.465780	0.083508
C	0.792402	0.297321	0.082236
C	0.724976	0.196206	0.085199
C	0.399303	0.299377	0.085153
C	0.575122	0.195725	0.086069
C	0.546585	0.689675	0.165299
C	0.376568	0.737769	0.168272
C	0.261443	0.685865	0.166061
C	0.239818	0.551164	0.166431
C	0.704594	0.544911	0.159681
C	0.788380	0.373524	0.163689
C	0.771517	0.235835	0.167547
C	0.324668	0.378691	0.167992
C	0.657703	0.181991	0.169520
C	0.486003	0.236138	0.169448
C	0.379214	0.737492	0.334534
C	0.706637	0.543785	0.324732
C	0.263309	0.685005	0.332508
C	0.240226	0.551090	0.332776
C	0.789297	0.372915	0.330413
C	0.771515	0.235734	0.334005
C	0.324592	0.378710	0.334301
C	0.657620	0.181972	0.335913
C	0.485923	0.236165	0.335788
C	0.549486	0.692787	0.331108
C	0.641562	0.627438	0.404755
C	0.459920	0.731379	0.417106

C	0.760309	0.458097	0.412488
C	0.312198	0.722155	0.416585
C	0.238564	0.626197	0.416039
C	0.792963	0.296965	0.415971
C	0.269824	0.465602	0.417129
C	0.725066	0.196181	0.418823
C	0.575216	0.195664	0.419732
C	0.399380	0.299223	0.418813
C	0.454756	0.737885	0.584869
C	0.662005	0.631369	0.562695
C	0.758878	0.459812	0.578947
C	0.791477	0.298137	0.582436
C	0.311953	0.721674	0.582676
C	0.575091	0.195678	0.586073
C	0.399283	0.299225	0.585148
C	0.724820	0.196372	0.585215
C	0.269706	0.465626	0.583505
C	0.238170	0.626261	0.582333
C	0.532421	0.725561	0.679986
C	0.485968	0.235958	0.669447
C	0.785767	0.375392	0.664004
C	0.713496	0.548799	0.658489
C	0.657542	0.182180	0.669549
C	0.324644	0.378551	0.668006
C	0.770397	0.236941	0.667641
C	0.239856	0.551006	0.666437
C	0.377141	0.738558	0.666107
C	0.262672	0.684918	0.665883
C	0.706515	0.550909	0.826754
C	0.485889	0.236026	0.835790
C	0.657456	0.182267	0.835912
C	0.785686	0.375977	0.830130
C	0.324583	0.378700	0.834334
C	0.374543	0.740087	0.832693
C	0.770184	0.237257	0.833941
C	0.239641	0.551225	0.832837
C	0.260906	0.686186	0.832338
C	0.541070	0.700345	0.838566
C	0.632079	0.631577	0.912279
C	0.756288	0.461837	0.910803
C	0.575184	0.195682	0.919742
C	0.399375	0.299224	0.918825
C	0.791070	0.298907	0.915747
C	0.724749	0.196687	0.918839
C	0.307820	0.725083	0.916185
C	0.269688	0.465639	0.917130

C	0.236652	0.627050	0.916034
C	0.454779	0.728288	0.919945
N	0.613576	0.725954	0.619996

TMS

a=10; b=10; c=10

$\alpha=90$; $\beta=90$; $\gamma=90$

Energy: -36.29769797 a.u.

k-grid dimension: (2x2x2)

Fractional Coordinates

H	0.170801	0.000124	-0.182224
H	0.230894	0.088747	-0.040516
H	0.230855	-0.088817	-0.040699
H	-0.193760	-0.158034	-0.023377
H	-0.091143	-0.163993	-0.168570
H	-0.039102	-0.245186	-0.019517
H	-0.193792	0.157956	-0.023562
H	-0.039180	0.245175	-0.019403
H	-0.090954	0.164056	-0.168590
H	-0.097697	-0.000067	0.228819
H	0.056156	-0.088814	0.226258
H	0.056050	0.088868	0.226261
C	0.004268	-0.000002	0.187188
C	0.174016	0.000009	-0.072138
C	-0.089575	0.155527	-0.058888
C	-0.089599	-0.155532	-0.058863
Si	-0.000436	-0.000001	-0.001072

Benzene

a=10; b=10; c=10

$\alpha=90$; $\beta=90$; $\gamma=90$

Energy: -38.28040414 a.u.

k-grid dimension: (2x2x2)

Fractional Coordinates

H	-0.214389	0.126544	0.000000
H	0.002465	0.248964	0.000000
H	0.216867	0.122233	0.000000
H	0.214388	-0.126546	0.000000
H	-0.002462	-0.248964	0.000000
H	-0.216868	-0.122231	0.000000
C	-0.121715	-0.068666	0.000000
C	-0.120318	0.071084	0.000000
C	0.001397	0.139769	0.000000
C	0.121715	0.068666	0.000000

C 0.120318 -0.071084 0.000000
C -0.001397 -0.139769 0.000000

NH

a=10; b=10; c=10

$\alpha=90$; $\beta=90$; $\gamma=90$

Energy: -10.49501238 a.u.

k-grid dimension: (4x4x4)

Fractional Coordinates

H	1	0.102958	0.000000	0.000000
N	1	-0.002958	0.000000	0.000000

NCH₃

a=10; b=10; c=10

$\alpha=90$; $\beta=90$; $\gamma=90$

Energy: -17.49321414 a.u.

k-grid dimension: (4x4x4)

Fractional Coordinates

H	1	0.536113	0.332190	0.353290
H	2	0.582998	0.481734	0.440392
H	3	0.537911	0.334533	0.532524
C	1	0.590358	0.371080	0.441871
N	1	0.725737	0.329479	0.441065

NCH₂OH

a=10; b=10; c=10

$\alpha=90$; $\beta=90$; $\gamma=90$

Energy: -33.66268583 a.u.

k-grid dimension: (5x5x5)

Fractional Coordinates

H	1	0.724965	0.321269	0.532857
H	2	0.564649	0.488009	0.370015
H	3	0.525335	0.209617	0.361095
C	1	0.572562	0.389067	0.417145
N	1	0.703391	0.340069	0.432581
O	1	0.483445	0.297911	0.361207

CH₂NHCH₂

a=10; b=10; c=10

$\alpha=90$; $\beta=90$; $\gamma=90$

Energy: -24.45871078 a.u.

k-grid dimension: (4x4x4)

Fractional Coordinates

H	1	0.689169	0.251685	0.217234
H	2	0.579280	0.378550	0.305032
H	3	0.722960	0.143896	0.426203

H	4	0.582673	0.376474	0.554777
H	5	0.699107	0.251157	0.636383
C	1	0.650322	0.296273	0.308405
C	2	0.655100	0.295635	0.547533
N	1	0.656508	0.221543	0.427709