

Supporting Information Available

DFT study of ionic peapod structures from single-walled carbon nanotubes and Lindqvist tungstates

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The material enclosed in the supporting information is organized as following:

1. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (9,9) h-CNT with various methods in Table S1-S5.
2. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (8,8) h-CNT with various methods in Table S6-S10.
3. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT for optimized $W_6O_{19}^{2-}@ (10,10)$ h-CNT with BLYPGrimme3 method in Table S11.
4. Coordinates (xyz) for various y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (n,n) h-CNT (n = 8, 9, 10).

Table S1. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (9,9) h-CNT with LDA method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-140.02	-170.26	291.78	-18.49
15°/0°	-129.06	-142.41	235.68	-35.79
30°/0°	-114.98	-98.84	156.54	-57.29
45°/0°	-110.97	-82.63	131.84	-61.76
45°/15°	-99.74	-57.74	78.90	-78.59
45°/30°	-90.72	-29.33	21.19	-98.86
45°/45°	-92.55	-35.54	32.30	-95.79
45°/60°	-106.39	-80.13	114.03	-72.49
45°/75°	-133.38	-148.09	248.03	-33.43
45°/90°	-139.77	-169.96	290.98	-18.75
45°/36 ^{oa}	-93.62	-40.38	25.42	-108.58

^a The orientation is based on the fully optimized structure.

Table S2. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (9,9) h-CNT with OPBE method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-175.38	-150.94	378.52	52.21
15°/0°	-164.58	-124.15	321.97	33.24
30°/0°	-152.22	-82.58	240.55	5.74
45°/0°	-149.75	-67.21	213.86	-3.10
45°/15°	-138.20	-43.15	162.31	-19.03
45°/30°	-129.38	-16.04	106.27	-39.15
45°/45°	-130.95	-21.96	117.34	-35.58
45°/60°	-143.07	-64.44	199.34	-8.17
45°/75°	-169.22	-129.76	334.04	35.06
45°/90°	-175.12	-150.65	377.74	51.97
45°/36 ^{oa}	-129.75	-14.28	98.68	-45.34

^a The orientation is based on the fully optimized structure.

Table S3. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (9,9) h-CNT with BP86 method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-141.66	-170.01	354.11	42.44
15°/0°	-131.30	-142.47	296.02	22.25
30°/0°	-118.21	-99.42	212.47	-5.16
45°/0°	-114.60	-83.42	185.39	-12.64
45°/15°	-103.86	-58.76	131.37	-31.25
45°/30°	-95.46	-30.71	71.83	-54.33
45°/45°	-97.14	-36.86	83.52	-50.48
45°/60°	-109.99	-80.91	169.37	-21.52
45°/75°	-135.60	-148.17	308.31	24.54
45°/90°	-141.41	-169.75	353.34	42.18
45°/36 ^{oa}	-94.46	-31.35	66.88	-58.92

^a The orientation is based on the fully optimized structure.

Table S4. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (9,9) h-CNT with BLYP method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-132.22	-178.20	378.37	67.95
15°/0°	-122.17	-150.49	318.61	45.95
30°/0°	-109.58	-107.16	231.68	14.94
45°/0°	-106.18	-90.95	202.84	5.71
45°/15°	-95.77	-66.30	147.75	-14.32
45°/30°	-87.63	-38.15	86.41	-39.37
45°/45°	-89.25	-44.31	98.58	-34.98
45°/60°	-101.54	-88.67	187.85	-2.36
45°/75°	-126.32	-156.14	330.84	48.38
45°/90°	-132.01	-177.85	377.55	67.68
45°/36 ^{oa}	-85.34	-35.16	77.54	-42.97

^a The orientation is based on the fully optimized structure.

Table S5. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (9,9) h-CNT with BLYPGrimme3 method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{disp}	ΔE_{int}
0°/0°	-132.22	-178.20	378.37	-96.52	-28.57
15°/0°	-122.17	-150.49	318.61	-96.78	-50.83
30°/0°	-109.58	-107.16	231.68	-96.64	-81.70
45°/0°	-106.18	-90.95	202.84	-95.70	-89.99
45°/15°	-95.77	-66.30	147.75	-97.03	-111.35
45°/30°	-87.63	-38.15	86.41	-100.18	-139.55
45°/45°	-89.25	-44.31	98.58	-99.63	-134.61
45°/60°	-101.54	-88.67	187.85	-97.88	-100.25
45°/75°	-126.32	-156.14	330.84	-97.11	-48.73
45°/90°	-132.01	-177.85	377.55	-96.51	-28.83
45°/36° ^a	-87.05	-40.50	86.13	-105.10	-146.52

^a The orientation is based on the fully optimized structure.

Table S6. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (8,8) h-CNT with LDA method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-667.46	-953.58	2066.10	445.06
15°/0°	-564.53	-833.23	1764.26	366.49
30°/0°	-428.45	-625.94	1272.28	217.89
45°/0°	-390.99	-542.19	1090.96	157.79
45°/15°	-293.81	-439.33	819.94	86.80
45°/30°	-179.53	-292.98	446.83	-25.68
45°/45°	-208.02	-336.66	548.45	3.77
45°/60°	-354.51	-562.47	1089.23	172.25
45°/75°	-579.55	-832.40	1760.23	348.28
45°/90°	-666.11	-952.48	2063.04	444.46
45°/39° ^a	-129.38	-184.72	212.95	-101.16

^a The orientation is based on the fully optimized structure.

Table S7. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (8,8) h-CNT with OPBE method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-713.61	-916.78	2184.03	553.64
15°/0°	-611.06	-797.63	1885.79	477.10
30°/0°	-474.82	-594.46	1403.61	334.32
45°/0°	-438.09	-513.51	1228.27	276.67
45°/15°	-339.25	-410.83	960.90	210.83
45°/30°	-221.57	-265.99	595.21	107.66
45°/45°	-251.14	-308.75	693.85	133.96
45°/60°	-400.41	-530.14	1221.42	290.87
45°/75°	-626.54	-796.47	1882.02	459.01
45°/90°	-712.18	-915.83	2181.07	553.06
45°/39° ^{aa}	-166.06	-141.91	324.22	16.24

^a The orientation is based on the fully optimized structure.

Table S8. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (8,8) h-CNT with BP86 method

Orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-654.82	-947.37	2181.79	579.60
15°/0°	-554.41	-827.64	1877.72	495.66
30°/0°	-422.43	-621.93	1380.39	336.03
45°/0°	-386.69	-539.02	1195.69	269.98
45°/15°	-291.41	-436.58	924.21	196.21
45°/30°	-179.66	-291.14	550.17	79.37
45°/45°	-207.48	-334.48	652.35	110.39
45°/60°	-349.73	-558.56	1197.49	289.20
45°/75°	-569.56	-826.88	1873.99	477.56
45°/90°	-653.49	-946.28	2178.73	578.96
45°/39° ^{aa}	-125.25	-158.90	266.23	-17.92

^a The orientation is based on the fully optimized structure.

Table S9. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (8,8) h-CNT with BLYP method

orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{int}
0°/0°	-634.84	-955.26	2240.82	650.72
15°/0°	-535.83	-835.95	1934.52	562.74
30°/0°	-406.47	-630.62	1431.54	394.46
45°/0°	-371.68	-547.64	1243.31	323.98
45°/15°	-277.77	-445.76	971.04	247.51
45°/30°	-168.15	-300.98	595.31	126.18
45°/45°	-195.31	-344.16	698.28	158.81
45°/60°	-334.40	-567.66	1248.67	346.62
45°/75°	-551.16	-835.29	1930.89	544.45
45°/90°	-633.53	-954.15	2237.72	650.05
45°/39° ^a	-112.82	-158.17	285.82	14.83

^a The orientation is based on the fully optimized structure.

Table S10. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT at different y/z orientations of $W_6O_{19}^{2-}$ encapsulated in (8,8) h-CNT with BLYPGrimme3 method

Orientations	ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{disp}	ΔE_{int}
0°/0°	-634.84	-955.26	2240.82	-126.00	524.72
15°/0°	-535.83	-835.95	1934.52	-129.76	432.98
30°/0°	-406.47	-630.62	1431.54	-141.45	253.01
45°/0°	-371.68	-547.64	1243.31	-150.33	173.65
45°/15°	-277.77	-445.76	971.04	-152.55	94.96
45°/30°	-168.15	-300.98	595.31	-158.04	-31.86
45°/45°	-195.31	-344.16	698.28	-155.42	3.39
45°/60°	-334.40	-567.66	1248.67	-140.26	206.35
45°/75°	-551.16	-835.29	1930.89	-130.39	414.06
45°/90°	-633.53	-954.15	2237.72	-126.02	524.03
45°/39° ^a	-113.65	-163.33	293.82	-163.05	-146.21

^a The orientation is based on the fully optimized structure.

Table S11. Energy decomposition analysis (in kcal/mol) of interaction between POM and h-CNT for optimized $W_6O_{19}^{2-}@ (10,10)$ h-CNT with BLYPGrimme3 method

ΔE_{orb}	ΔE_{elstat}	ΔE_{Pauli}	ΔE_{disp}	ΔE_{int}
-71.89	-31.30	77.72	-76.18	-101.65

Coordinates (xyz)

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 0°/0°)

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C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989

C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082

C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894

C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428

C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412

H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	0.00001	-0.00001	-0.00001
W	2.32689	0.00000	-0.00000
W	-2.32689	-0.00001	-0.00001
W	0.00000	0.00000	2.32687
W	-0.00000	0.00001	-2.32686
W	-0.00001	-2.32686	0.00000
W	0.00001	2.32687	0.00001
O	1.88436	1.88435	0.00000
O	-1.88434	1.88432	0.00001
O	-1.88436	-1.88435	-0.00001
O	1.88435	-1.88433	-0.00001
O	1.88435	-0.00000	-1.88436
O	1.88435	-0.00000	1.88435
O	-1.88434	-0.00002	1.88435
O	-1.88435	-0.00001	-1.88435
O	-0.00001	-1.88437	-1.88437
O	-0.00001	-1.88438	1.88438
O	0.00000	1.88438	1.88438
O	-0.00000	1.88438	-1.88437
O	-0.00001	0.00005	4.04246
O	-0.00002	0.00000	-4.04246
O	0.00002	4.04246	-0.00001
O	-0.00001	-4.04246	0.00003
O	4.04250	0.00002	0.00000
O	-4.04250	-0.00002	-0.00000

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 15°/0°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610

C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230

C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738

C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984

C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762

H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	0.00000	-0.00001	-0.00001
W	2.24760	0.00000	-0.60225
W	-2.24760	-0.00001	0.60223
W	0.60224	0.00000	2.24758
W	-0.60224	0.00001	-2.24757
W	-0.00001	-2.32686	0.00000
W	0.00001	2.32687	0.00000
O	1.82015	1.88435	-0.48770
O	-1.82013	1.88432	0.48771
O	-1.82015	-1.88435	0.48770
O	1.82014	-1.88433	-0.48772
O	1.33244	-0.00000	-2.30785
O	2.30785	-0.00000	1.33244
O	-1.33243	-0.00002	2.30784
O	-2.30785	-0.00001	-1.33244
O	-0.48772	-1.88437	-1.82016
O	0.48771	-1.88438	1.82017
O	0.48772	1.88438	1.82017
O	-0.48771	1.88438	-1.82016
O	1.04626	0.00005	3.90472
O	-1.04629	0.00000	-3.90471
O	0.00001	4.04246	-0.00002
O	-0.00000	-4.04246	0.00003
O	3.90475	0.00002	-1.04627
O	-3.90476	-0.00002	1.04627

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 30°/0°)

217

C	-4.30492	1.42279	-5.32884
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C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145

C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523

C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546

C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034

C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381

H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	0.00000	-0.00001	-0.00001
W	2.01514	0.00000	-1.16345
W	-2.01515	-0.00001	1.16344
W	1.16343	0.00000	2.01512
W	-1.16343	0.00001	-2.01512
W	-0.00001	-2.32686	0.00000
W	0.00001	2.32687	-0.00000
O	1.63191	1.88435	-0.94218
O	-1.63188	1.88432	0.94218
O	-1.63190	-1.88435	0.94217
O	1.63189	-1.88433	-0.94218
O	0.68972	-0.00000	-2.57408
O	2.57407	-0.00000	0.68972
O	-0.68972	-0.00002	2.57406
O	-2.57407	-0.00001	-0.68972
O	-0.94220	-1.88437	-1.63191
O	0.94218	-1.88438	1.63192
O	0.94219	1.88438	1.63192
O	-0.94219	1.88438	-1.63191
O	2.02122	0.00005	3.50088
O	-2.02125	0.00000	-3.50086
O	0.00001	4.04246	-0.00002
O	0.00000	-4.04246	0.00003
O	3.50091	0.00002	-2.02125
O	-3.50091	-0.00002	2.02125

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/0°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063

C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679

C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116

C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364

C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066

C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268

H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	-0.00000	-0.00001	-0.00001
W	1.64535	0.00000	-1.64536
W	-1.64536	-0.00001	1.64535
W	1.64534	0.00000	1.64534
W	-1.64534	0.00001	-1.64534
W	-0.00000	-2.32686	0.00000
W	0.00001	2.32687	-0.00001
O	1.33245	1.88435	-1.33244
O	-1.33242	1.88432	1.33243
O	-1.33245	-1.88435	1.33243
O	1.33243	-1.88433	-1.33244
O	-0.00001	-0.00000	-2.66488
O	2.66487	-0.00000	-0.00000
O	0.00000	-0.00002	2.66487
O	-2.66487	-0.00001	0.00000
O	-1.33246	-1.88437	-1.33244
O	1.33245	-1.88438	1.33246
O	1.33246	1.88438	1.33246
O	-1.33245	1.88438	-1.33245
O	2.85844	0.00005	2.85846
O	-2.85847	0.00000	-2.85843
O	0.00000	4.04246	-0.00002
O	0.00001	-4.04246	0.00003
O	2.85848	0.00002	-2.85848
O	-2.85848	-0.00002	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/15°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810

C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004

C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040

C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433

C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859

C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993

H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	-0.00000	-0.00000	-0.00001
W	1.58929	-0.42585	-1.64536
W	-1.58930	0.42584	1.64535
W	1.58928	-0.42584	1.64534
W	-1.58928	0.42585	-1.64534
W	-0.60224	-2.24758	0.00000
W	0.60225	2.24758	-0.00001
O	1.77475	1.47528	-1.33244
O	-0.79932	2.16497	1.33243
O	-1.77475	-1.47528	1.33244
O	0.79932	-2.16498	-1.33244
O	-0.00001	-0.00000	-2.66488
O	2.57407	-0.68972	-0.00000
O	-0.00000	-0.00002	2.66487
O	-2.57407	0.68971	0.00000
O	-1.77477	-1.47530	-1.33244
O	0.79934	-2.16504	1.33246
O	1.77477	1.47531	1.33245
O	-0.79934	2.16504	-1.33245
O	2.76106	-0.73978	2.85846
O	-2.76107	0.73983	-2.85843
O	1.04627	3.90472	-0.00002
O	-1.04625	-3.90472	0.00003
O	2.76108	-0.73981	-2.85848
O	-2.76108	0.73981	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/30°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881

C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230

C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722

C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043

C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482

C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683

O	-0.00000	-0.00000	-0.00001
W	1.42492	-0.82268	-1.64536
W	-1.42493	0.82267	1.64535
W	1.42491	-0.82267	1.64534
W	-1.42491	0.82268	-1.64534
W	-1.16344	-2.01512	0.00000
W	1.16344	2.01512	-0.00001
O	2.09611	0.96567	-1.33244
O	-0.21175	2.29808	1.33243
O	-2.09611	-0.96567	1.33244
O	0.21175	-2.29809	-1.33244
O	-0.00001	-0.00000	-2.66488
O	2.30785	-1.33244	-0.00000
O	-0.00001	-0.00002	2.66487
O	-2.30785	1.33243	0.00000
O	-2.09613	-0.96568	-1.33244
O	0.21175	-2.29815	1.33246
O	2.09614	0.96569	1.33245
O	-0.21175	2.29815	-1.33245
O	2.47551	-1.42918	2.85846
O	-2.47551	1.42923	-2.85843
O	2.02123	3.50087	-0.00002
O	-2.02122	-3.50088	0.00003
O	2.47552	-1.42922	-2.85848
O	-2.47552	1.42923	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/45°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697

C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646

C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259

C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594

C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462

C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	-0.00000	-0.00000	-0.00001
W	1.16344	-1.16344	-1.64536

W	-1.16346	1.16344	1.64535
W	1.16344	-1.16343	1.64534
W	-1.16343	1.16344	-1.64534
W	-1.64535	-1.64534	0.00000
W	1.64535	1.64533	-0.00001
O	2.27462	0.39025	-1.33244
O	0.39026	2.27458	1.33243
O	-2.27462	-0.39025	1.33244
O	-0.39026	-2.27459	-1.33244
O	-0.00001	0.00000	-2.66488
O	1.88435	-1.88435	-0.00000
O	-0.00001	-0.00002	2.66487
O	-1.88435	1.88435	0.00000
O	-2.27465	-0.39026	-1.33244
O	-0.39027	-2.27464	1.33246
O	2.27466	0.39027	1.33245
O	0.39027	2.27465	-1.33245
O	2.02126	-2.02119	2.85846
O	-2.02124	2.02124	-2.85843
O	2.85845	2.85845	-0.00002
O	-2.85844	-2.85846	0.00003
O	2.02126	-2.02124	-2.85848
O	-2.02126	2.02124	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/60°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525

C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811

C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410

C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684

C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149

C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	-0.00001	-0.00000	-0.00001
W	0.82268	-1.42492	-1.64536
W	-0.82269	1.42492	1.64535
W	0.82267	-1.42491	1.64534

W	-0.82267	1.42491	-1.64534
W	-2.01513	-1.16343	0.00000
W	2.01513	1.16342	-0.00001
O	2.29811	-0.21176	-1.33244
O	0.96566	2.09607	1.33243
O	-2.29812	0.21176	1.33244
O	-0.96567	-2.09608	-1.33244
O	-0.00001	0.00000	-2.66488
O	1.33244	-2.30785	-0.00000
O	-0.00001	-0.00001	2.66487
O	-1.33244	2.30785	0.00000
O	-2.29815	0.21176	-1.33244
O	-0.96570	-2.09613	1.33246
O	2.29816	-0.21175	1.33245
O	0.96570	2.09613	-1.33245
O	1.42926	-2.47546	2.85846
O	-1.42923	2.47551	-2.85843
O	3.50088	2.02123	-0.00002
O	-3.50087	-2.02124	0.00003
O	1.42925	-2.47551	-2.85848
O	-1.42925	2.47551	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/75°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225

C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752
C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894

C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642
C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457

C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146
C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884

C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740
C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616

H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933
H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	-0.00001	-0.00000	-0.00001
W	0.42585	-1.58929	-1.64536
W	-0.42586	1.58930	1.64535
W	0.42585	-1.58928	1.64534
W	-0.42584	1.58928	-1.64534
W	-2.24758	-0.60223	0.00000

W	2.24759	0.60222	-0.00001
O	2.16500	-0.79934	-1.33244
O	1.47526	1.77472	1.33243
O	-2.16500	0.79934	1.33244
O	-1.47527	-1.77473	-1.33244
O	-0.00001	0.00000	-2.66488
O	0.68972	-2.57407	-0.00000
O	-0.00002	-0.00001	2.66487
O	-0.68972	2.57407	0.00000
O	-2.16503	0.79935	-1.33244
O	-1.47531	-1.77476	1.33246
O	2.16504	-0.79935	1.33245
O	1.47531	1.77477	-1.33245
O	0.73987	-2.76104	2.85846
O	-0.73983	2.76107	-2.85843
O	3.90472	1.04626	-0.00002
O	-3.90471	-1.04627	0.00003
O	0.73984	-2.76108	-2.85848
O	-0.73984	2.76108	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/90°)

217

C	-4.30492	1.42279	-5.32884
C	-1.84686	1.40599	-5.23837
C	0.60489	1.40776	-5.25063
C	3.06853	1.41116	-5.26147
C	5.47690	1.51187	-5.43810
C	-4.30631	2.75755	-4.77487
C	-1.84825	2.70933	-4.69881
C	0.60347	2.72095	-4.70735
C	3.06709	2.72975	-4.71697
C	5.47524	2.78648	-4.91323
C	-5.49321	3.46066	-4.43525
C	-3.08381	3.30912	-4.31728
C	-0.62004	3.30923	-4.31225
C	1.83186	3.31044	-4.30597
C	4.28923	3.36592	-4.38752

C	-5.49317	4.43489	-3.46026
C	-3.08374	4.31783	-3.30835
C	-0.62001	4.31537	-3.30851
C	1.83175	4.30859	-3.30933
C	4.28952	4.38688	-3.36491
C	-4.30656	4.77367	-2.75649
C	-1.84841	4.70145	-2.70903
C	0.60341	4.71146	-2.72066
C	3.06729	4.71865	-2.72900
C	5.47638	4.90874	-2.78409
C	-4.30573	5.32580	-1.42098
C	-1.84727	5.24066	-1.40552
C	0.60450	5.25403	-1.40707
C	3.06841	5.26287	-1.41030
C	5.47739	5.43350	-1.50982
C	-5.49160	5.58314	-0.68197
C	-3.08190	5.39401	-0.70960
C	-0.61782	5.39031	-0.70989
C	1.83403	5.38428	-0.70757
C	4.29213	5.47355	-0.72798
C	-5.48939	5.58319	0.69610
C	-3.07991	5.39336	0.71720
C	-0.61585	5.38964	0.71145
C	1.83580	5.38343	0.70305
C	4.29400	5.47258	0.71679
C	-4.30176	5.32594	1.43173
C	-1.84357	5.23931	1.41004
C	0.60816	5.25225	1.40546
C	3.07206	5.26124	1.40230
C	5.48165	5.43084	1.49523
C	-4.29962	4.77238	2.76646
C	-1.84134	4.69988	2.71369
C	0.61046	4.70728	2.71811
C	3.07424	4.71503	2.72027
C	5.48374	4.90443	2.76894
C	-5.48473	4.43360	3.47317
C	-3.07539	4.31763	3.31642

C	-0.61146	4.31279	3.30999
C	1.84017	4.30413	3.30370
C	4.29822	4.38172	3.35198
C	-5.48254	3.46099	4.44958
C	-3.07286	3.30948	4.32597
C	-0.60906	3.30799	4.31532
C	1.84230	3.30648	4.30118
C	4.30032	3.35873	4.37240
C	-4.29452	2.75816	4.78625
C	-1.83664	2.70922	4.70535
C	0.61480	2.71839	4.70760
C	3.07845	2.72456	4.70786
C	5.48790	2.77789	4.89254
C	-4.29209	1.42316	5.33900
C	-1.83470	1.40552	5.24437
C	0.61664	1.40540	5.25220
C	3.08048	1.40636	5.25366
C	5.48985	1.50493	5.42082
C	-5.47754	0.68550	5.59987
C	-3.06919	0.71055	5.40178
C	-0.60571	0.70885	5.39230
C	1.84593	0.70460	5.37929
C	4.30417	0.72353	5.46523
C	-5.47719	-0.69272	5.59886
C	-3.06856	-0.71631	5.40116
C	-0.60484	-0.71251	5.39188
C	1.84687	-0.70616	5.38040
C	4.30530	-0.72143	5.46684
C	-4.29111	-1.42970	5.33722
C	-1.83322	-1.41046	5.24440
C	0.61848	-1.40765	5.25259
C	3.08275	-1.40632	5.25668
C	5.49216	-1.50137	5.42410
C	-4.29104	-2.76477	4.78395
C	-1.83299	-2.71379	4.70457
C	0.61877	-2.72063	4.70851
C	3.08306	-2.72461	4.71146

C	5.49261	-2.77447	4.89610
C	-5.47753	-3.46988	4.44663
C	-3.06854	-3.31486	4.32442
C	-0.60446	-3.31106	4.31512
C	1.84757	-3.30743	4.30373
C	4.30572	-3.35729	4.37663
C	-5.47802	-4.44296	3.47029
C	-3.06910	-4.32254	3.31424
C	-0.60521	-4.31588	3.31005
C	1.84678	-4.30426	3.30554
C	4.30463	-4.37834	3.35454
C	-4.29214	-4.78040	2.76454
C	-1.83428	-4.70336	2.71222
C	0.61763	-4.70864	2.71930
C	3.08153	-4.71206	2.72181
C	5.49093	-4.89773	2.77107
C	-4.29283	-5.33340	1.42964
C	-1.83502	-5.24311	1.40894
C	0.61666	-5.25177	1.40580
C	3.08067	-5.25697	1.40344
C	5.49031	-5.42380	1.49738
C	-5.48007	-5.59232	0.69381
C	-3.07075	-5.39876	0.71546
C	-0.60695	-5.39089	0.71089
C	1.84488	-5.38073	0.70364
C	4.30313	-5.46761	0.71871
C	-5.48143	-5.58999	-0.68433
C	-3.07211	-5.39774	-0.71116
C	-0.60824	-5.39097	-0.71043
C	1.84371	-5.38190	-0.70708
C	4.30208	-5.46797	-0.72594
C	-4.29579	-5.33069	-1.42244
C	-1.83757	-5.24253	-1.40684
C	0.61442	-5.25258	-1.40707
C	3.07849	-5.25794	-1.40884
C	5.48819	-5.42281	-1.50651
C	-4.29727	-4.77837	-2.75740

C	-1.83885	-4.70357	-2.71051
C	0.61342	-4.70803	-2.71995
C	3.07767	-4.70985	-2.72595
C	5.48707	-4.89509	-2.77963
C	-5.48458	-4.44145	-3.46128
C	-3.07484	-4.32292	-3.31056
C	-0.61057	-4.31566	-3.30952
C	1.84155	-4.30237	-3.30755
C	4.29976	-4.37405	-3.36004
C	-5.48549	-3.46953	-4.43828
C	-3.07606	-3.31498	-4.32025
C	-0.61201	-3.31062	-4.31435
C	1.84020	-3.30461	-4.30489
C	4.29835	-3.35150	-4.38073
C	-4.29944	-2.76528	-4.77839
C	-1.84140	-2.71338	-4.70148
C	0.61045	-2.71900	-4.70799
C	3.07450	-2.72002	-4.71428
C	5.48384	-2.76804	-4.90322
C	-4.30124	-1.43013	-5.33115
C	-1.84337	-1.40944	-5.23984
C	0.60857	-1.40536	-5.25066
C	3.07239	-1.40170	-5.26034
C	5.48160	-1.49549	-5.43259
C	-5.48849	-0.69405	-5.59066
C	-3.07938	-0.71599	-5.39552
C	-0.61554	-0.71101	-5.38859
C	1.83606	-0.70235	-5.38122
C	4.29411	-0.71643	-5.47482
C	-5.49056	0.68435	-5.58884
C	-3.08138	0.71075	-5.39462
C	-0.61742	0.71031	-5.38818
C	1.83420	0.70836	-5.38149
C	4.29196	0.72887	-5.47594
H	6.42247	1.08806	-5.75616
H	6.41952	3.31363	-4.83975
H	-6.43890	3.18801	-4.88933

H	-6.43887	4.88844	-3.18673
H	6.42128	4.83340	-3.30980
H	6.42301	5.74980	-1.08485
H	-6.43814	5.71049	-1.19460
H	-6.43445	5.71047	1.21147
H	6.42636	5.74728	1.06829
H	6.42992	4.82777	3.29224
H	-6.43107	4.88709	3.20187
H	-6.42711	3.18839	4.90611
H	6.43279	3.30298	4.81342
H	6.43626	1.08070	5.73584
H	-6.42299	1.19919	5.73038
H	-6.42239	-1.20712	5.72850
H	6.43775	-1.07492	5.73860
H	6.43850	-3.29789	4.81718
H	-6.42269	-3.19825	4.90249
H	-6.42359	-4.89776	3.19851
H	6.43697	-4.81866	3.29412
H	6.43579	-5.73758	1.07027
H	-6.42500	-5.72179	1.20886
H	-6.42744	-5.71830	-1.19762
H	6.43444	-5.73728	-1.08156
H	6.43240	-4.81493	-3.30381
H	-6.42975	-4.89535	-3.18705
H	-6.43134	-3.19802	-4.89268
H	6.43035	-3.29062	-4.82609
H	6.42636	-1.06916	-5.74993
H	-6.43318	-1.20942	-5.72020
H	-6.43683	1.19729	-5.71683
O	-0.00001	0.00000	-0.00001
W	0.00000	-1.64536	-1.64536
W	-0.00001	1.64537	1.64535
W	0.00000	-1.64535	1.64534
W	0.00001	1.64534	-1.64534
W	-2.32687	0.00001	0.00000
W	2.32687	-0.00001	-0.00001
O	1.88435	-1.33245	-1.33244

O	1.88433	1.33242	1.33243
O	-1.88435	1.33245	1.33244
O	-1.88434	-1.33243	-1.33244
O	-0.00001	0.00000	-2.66488
O	-0.00000	-2.66488	-0.00000
O	-0.00002	-0.00000	2.66487
O	-0.00000	2.66488	0.00000
O	-1.88438	1.33247	-1.33244
O	-1.88438	-1.33245	1.33246
O	1.88439	-1.33246	1.33245
O	1.88439	1.33245	-1.33245
O	0.00005	-2.85845	2.85846
O	-0.00000	2.85847	-2.85843
O	4.04246	-0.00001	-0.00002
O	-4.04246	-0.00001	0.00003
O	0.00001	-2.85848	-2.85848
O	-0.00001	2.85848	2.85848

W₆O₁₉²⁻@(8,8) h-CNT (y/z = 45°/39°)

217

C	-4.294787	1.506703	-5.436725
C	-1.828680	1.475462	-5.379228
C	0.621898	1.396144	-5.257269
C	3.082130	1.338020	-5.175802
C	5.505370	1.382048	-5.234057
C	-4.282270	2.873045	-4.963825
C	-1.816334	2.813083	-4.884106
C	0.631646	2.707369	-4.695652
C	3.090878	2.638989	-4.576374
C	5.513563	2.629454	-4.651678
C	-5.482756	3.546987	-4.591715
C	-3.058016	3.431674	-4.513994
C	-0.592398	3.359635	-4.395431
C	1.855043	3.256800	-4.218150
C	4.316290	3.253085	-4.204095
C	-5.498347	4.443732	-3.552272
C	-3.077520	4.361794	-3.417252

C	-0.609676	4.345730	-3.356460
C	1.840239	4.302577	-3.262445
C	4.299808	4.343250	-3.252318
C	-4.312515	4.731651	-2.818197
C	-1.854125	4.696931	-2.760270
C	0.598365	4.742645	-2.726129
C	3.064244	4.753353	-2.680614
C	5.484486	4.902939	-2.698045
C	-4.334478	5.150125	-1.433050
C	-1.873445	5.148556	-1.416825
C	0.576424	5.323935	-1.417114
C	3.040403	5.428087	-1.413805
C	5.464668	5.542846	-1.482252
C	-5.535102	5.291083	-0.682931
C	-3.113017	5.226105	-0.712729
C	-0.653581	5.355904	-0.712050
C	1.794232	5.565568	-0.715860
C	4.261026	5.661471	-0.729173
C	-5.533949	5.291180	0.694280
C	-3.111685	5.227225	0.720108
C	-0.651845	5.356621	0.714346
C	1.796349	5.564984	0.711775
C	4.264034	5.656024	0.716303
C	-4.332072	5.150645	1.442251
C	-1.870711	5.151257	1.422203
C	0.580046	5.323568	1.416575
C	3.044849	5.424390	1.405442
C	5.470884	5.525780	1.461802
C	-4.307463	4.730310	2.826511
C	-1.848557	4.698205	2.765224
C	0.604573	4.742904	2.726111
C	3.070950	4.749391	2.672336
C	5.493159	4.883417	2.676254
C	-5.492327	4.439973	3.561311
C	-3.071051	4.360275	3.422809
C	-0.602634	4.345666	3.358605
C	1.847757	4.301332	3.259017

C	4.307600	4.335397	3.239616
C	-5.474415	3.543788	4.601018
C	-3.049316	3.428776	4.518387
C	-0.583682	3.357511	4.396074
C	1.863622	3.254394	4.214147
C	4.324570	3.248654	4.194603
C	-4.272849	2.870497	4.971023
C	-1.806920	2.810161	4.885903
C	0.640950	2.704579	4.694053
C	3.099849	2.635756	4.569981
C	5.522685	2.624923	4.639558
C	-4.284530	1.505061	5.446777
C	-1.818189	1.473570	5.384537
C	0.632328	1.394020	5.258640
C	3.092328	1.334706	5.169808
C	5.516243	1.375873	5.218238
C	-5.491785	0.760868	5.574331
C	-3.066817	0.776527	5.478379
C	-0.604117	0.730421	5.457847
C	1.848627	0.662180	5.373797
C	4.310466	0.642930	5.400870
C	-5.510107	-0.606405	5.429456
C	-3.088216	-0.649984	5.329250
C	-0.626407	-0.701440	5.413962
C	1.826117	-0.752742	5.477650
C	4.284000	-0.792738	5.569806
C	-4.321077	-1.336976	5.158064
C	-1.861055	-1.364724	5.174561
C	0.584307	-1.437269	5.328339
C	3.052169	-1.487107	5.437341
C	5.473612	-1.578050	5.586691
C	-4.324493	-2.651580	4.552069
C	-1.863494	-2.659630	4.597932
C	0.580292	-2.769404	4.798615
C	3.046699	-2.840928	4.945984
C	5.470182	-2.864720	5.111548
C	-5.515051	-3.320442	4.157487

C	-3.092260	-3.241162	4.161169
C	-0.633628	-3.312242	4.300664
C	1.815745	-3.408675	4.477293
C	4.278766	-3.444209	4.582287
C	-5.493763	-4.362971	3.259386
C	-3.068712	-4.322202	3.220556
C	-0.608013	-4.346404	3.314895
C	1.844856	-4.348437	3.407154
C	4.309752	-4.352760	3.458539
C	-4.280203	-4.819641	2.673244
C	-1.817392	-4.766219	2.689929
C	0.636254	-4.737824	2.760613
C	3.097169	-4.664840	2.790056
C	5.523043	-4.717989	2.810020
C	-4.244176	-5.532881	1.416768
C	-1.785894	-5.402655	1.419649
C	0.664502	-5.239162	1.419965
C	3.122431	-5.082785	1.418718
C	5.545102	-5.115804	1.493369
C	-5.432334	-5.842000	0.690495
C	-3.011725	-5.650994	0.722852
C	-0.545888	-5.476437	0.717418
C	1.895365	-5.249311	0.707147
C	4.355538	-5.189012	0.719476
C	-5.434024	-5.839303	-0.680620
C	-3.013109	-5.650611	-0.718189
C	-0.547271	-5.475524	-0.716256
C	1.894448	-5.248557	-0.710772
C	4.354752	-5.188326	-0.728231
C	-4.246953	-5.532232	-1.409565
C	-1.788489	-5.402272	-1.417050
C	0.662100	-5.237450	-1.420691
C	3.120400	-5.081783	-1.424896
C	5.543219	-5.112665	-1.504028
C	-4.284887	-4.822158	-2.667763
C	-1.821974	-4.767285	-2.687936
C	0.631951	-4.736578	-2.761502

C	3.093041	-4.661945	-2.795623
C	5.518964	-4.713621	-2.820418
C	-5.499436	-4.364833	-3.251175
C	-3.074488	-4.324860	-3.217395
C	-0.613450	-4.346812	-3.314305
C	1.839480	-4.345868	-3.409882
C	4.304364	-4.348684	-3.466519
C	-5.522412	-3.321618	-4.148434
C	-3.099697	-3.242918	-4.156974
C	-0.640858	-3.312045	-4.298987
C	1.808392	-3.405896	-4.479681
C	4.271392	-3.439258	-4.589902
C	-4.332625	-2.652507	-4.544903
C	-1.871537	-2.659521	-4.592626
C	0.571880	-2.767817	-4.797887
C	3.038109	-2.837223	-4.951295
C	5.461439	-2.860012	-5.123204
C	-4.330514	-1.336364	-5.147800
C	-1.870460	-1.363247	-5.165836
C	0.574525	-1.434647	-5.323855
C	3.042133	-1.483596	-5.442335
C	5.463016	-1.574168	-5.600866
C	-5.520070	-0.605354	-5.416410
C	-3.098117	-0.648665	-5.318495
C	-0.636433	-0.699282	-5.405227
C	1.815759	-0.749976	-5.476287
C	4.273661	-0.788627	-5.578690
C	-5.502066	0.762025	-5.561038
C	-3.077128	0.777974	-5.468396
C	-0.614806	0.732169	-5.451115
C	1.838049	0.664752	-5.374095
C	4.299724	0.647357	-5.411535
H	6.458726	0.920200	-5.473546
H	6.472740	3.101187	-4.458594
H	-6.427318	3.263159	-5.048130
H	-6.451931	4.851057	-3.227145
H	6.441604	4.741586	-3.185942

H	6.409836	5.851839	-1.044556
H	-6.492045	5.313674	-1.196051
H	-6.490086	5.311652	1.208953
H	6.415350	5.831736	1.020483
H	6.451580	4.716423	3.159568
H	-6.446613	4.846894	3.237808
H	-6.417542	3.262157	5.061661
H	6.481292	3.096825	4.444411
H	6.470188	0.911816	5.451161
H	-6.439862	1.281289	5.675239
H	-6.470024	-1.115083	5.433655
H	6.419523	-1.126328	5.873465
H	6.414900	-3.395758	5.030507
H	-6.479158	-2.954156	4.498393
H	-6.442611	-4.771979	2.924369
H	6.471125	-4.584670	3.322864
H	6.508543	-5.288939	1.022574
H	-6.375499	-5.963051	1.216857
H	-6.378098	-5.961060	-1.205203
H	6.507775	-5.280666	-1.033892
H	6.466199	-4.573696	-3.333009
H	-6.447841	-4.771032	-2.911537
H	-6.487310	-2.953092	-4.484647
H	6.406519	-3.390736	-5.044153
H	6.407671	-1.122995	-5.892581
H	-6.479802	-1.114416	-5.421889
H	-6.450229	1.282275	-5.662253
O	-0.005618	-0.005285	0.001261
W	1.370853	-0.959035	-1.650206
W	-1.384807	0.941522	1.649442
W	1.372431	-0.963468	1.648676
W	-1.385643	0.945572	-1.644142
W	-1.388429	-1.918249	0.000129
W	1.375711	1.889642	0.003625
O	2.195177	0.765097	-1.342625
O	-0.003330	2.312457	1.347637
O	-2.201633	-0.786602	1.345849

O	-0.012088	-2.331007	-1.341853
O	-0.005745	-0.007475	-2.683002
O	2.184261	-1.568248	-0.001981
O	-0.004627	-0.016190	2.684830
O	-2.203934	1.549323	0.003385
O	-2.202289	-0.783563	-1.343781
O	-0.009790	-2.336255	1.336596
O	2.194788	0.762628	1.348608
O	-0.003468	2.316057	-1.339048
O	2.539364	-1.609473	2.743609
O	-2.548760	1.577527	-2.751456
O	2.537423	3.166483	0.004887
O	-2.565282	-3.181754	0.000343
O	2.534897	-1.603028	-2.749120
O	-2.549231	1.571158	2.757606

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 0°/0°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052

C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278

C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635

C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485

C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877

C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331

H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	0.00001	-0.00001	-0.00001
W	2.32689	-0.00150	0.00057
W	-2.32689	0.00149	-0.00058
W	-0.00057	0.00127	2.32687
W	0.00056	-0.00126	-2.32686
W	-0.00151	-2.32686	0.00127
W	0.00152	2.32686	-0.00126
O	1.88558	1.88313	-0.00056
O	-1.88312	1.88554	-0.00148
O	-1.88557	-1.88313	0.00056
O	1.88313	-1.88555	0.00148
O	1.88481	-0.00225	-1.88390
O	1.88389	-0.00019	1.88481
O	-1.88480	0.00223	1.88389
O	-1.88389	0.00018	-1.88481
O	-0.00077	-1.88540	-1.88334
O	-0.00168	-1.88335	1.88540
O	0.00076	1.88541	1.88335
O	0.00167	1.88336	-1.88540
O	-0.00100	0.00225	4.04246
O	0.00096	-0.00221	-4.04246
O	0.00263	4.04246	-0.00222
O	-0.00262	-4.04246	0.00224
O	4.04250	-0.00259	0.00099
O	-4.04250	0.00259	-0.00099

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 15°/0°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913

C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110

C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647

C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892

C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380

H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	0.00000	-0.00001	-0.00001
W	2.24775	-0.00150	-0.60170
W	-2.24775	0.00149	0.60168

W	0.60169	0.00127	2.24773
W	-0.60169	-0.00126	-2.24772
W	-0.00113	-2.32686	0.00162
W	0.00114	2.32686	-0.00161
O	1.82118	1.88313	-0.48857
O	-1.81934	1.88554	0.48596
O	-1.82118	-1.88313	0.48856
O	1.81934	-1.88555	-0.48596
O	1.33300	-0.00225	-2.30753
O	2.30752	-0.00019	1.33300
O	-1.33300	0.00223	2.30752
O	-2.30752	0.00018	-1.33300
O	-0.48819	-1.88540	-1.81897
O	0.48635	-1.88335	1.82160
O	0.48818	1.88541	1.81898
O	-0.48636	1.88336	-1.82159
O	1.04530	0.00225	3.90497
O	-1.04534	-0.00221	-3.90496
O	0.00197	4.04246	-0.00283
O	-0.00196	-4.04246	0.00284
O	3.90501	-0.00259	-1.04532
O	-3.90501	0.00259	1.04532

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 30°/0°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637

C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421

C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731

C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006

C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627

C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392

H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	0.00000	-0.00001	-0.00001
W	2.01543	-0.00150	-1.16295
W	-2.01543	0.00149	1.16294
W	1.16294	0.00127	2.01541
W	-1.16294	-0.00126	-2.01540
W	-0.00067	-2.32686	0.00186
W	0.00068	2.32686	-0.00185
O	1.63268	1.88313	-0.94328
O	-1.63157	1.88554	0.94028
O	-1.63267	-1.88313	0.94327
O	1.63158	-1.88555	-0.94028
O	0.69035	-0.00225	-2.57391
O	2.57390	-0.00019	0.69035
O	-0.69034	0.00223	2.57389
O	-2.57390	0.00018	-0.69035
O	-0.94234	-1.88540	-1.63064
O	0.94124	-1.88335	1.63365
O	0.94233	1.88541	1.63065

O	-0.94125	1.88336	-1.63364
O	2.02037	0.00225	3.50137
O	-2.02040	-0.00221	-3.50135
O	0.00117	4.04246	-0.00324
O	-0.00115	-4.04246	0.00325
O	3.50140	-0.00259	-2.02039
O	-3.50140	0.00259	2.02039

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/0°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932

C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099

C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385

C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027

C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788

C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878

H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00000	-0.00001	-0.00001
W	1.64576	-0.00150	-1.64496
W	-1.64577	0.00149	1.64495
W	1.64494	0.00127	1.64574
W	-1.64494	-0.00126	-1.64574
W	-0.00017	-2.32686	0.00197
W	0.00018	2.32686	-0.00197
O	1.33291	1.88313	-1.33370
O	-1.33261	1.88554	1.33052
O	-1.33291	-1.88313	1.33370
O	1.33262	-1.88555	-1.33053
O	0.00065	-0.00225	-2.66488
O	2.66487	-0.00019	0.00065
O	-0.00065	0.00223	2.66487
O	-2.66487	0.00018	-0.00065
O	-1.33227	-1.88540	-1.33118
O	1.33199	-1.88335	1.33437
O	1.33227	1.88541	1.33119
O	-1.33199	1.88336	-1.33436
O	2.85775	0.00225	2.85916
O	-2.85777	-0.00221	-2.85913
O	0.00029	4.04246	-0.00343
O	-0.00027	-4.04246	0.00344
O	2.85918	-0.00259	-2.85778
O	-2.85918	0.00259	2.85778

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/15°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889

C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151

C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914

C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956

C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319

C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488

H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00000	-0.00000	-0.00001
W	1.58929	-0.42740	-1.64496
W	-1.58930	0.42739	1.64495
W	1.58922	-0.42451	1.64574
W	-1.58922	0.42452	-1.64574
W	-0.60240	-2.24753	0.00197
W	0.60241	2.24753	-0.00197
O	1.77488	1.47398	-1.33370
O	-0.79919	2.16620	1.33052
O	-1.77488	-1.47398	1.33370
O	0.79919	-2.16621	-1.33053

O	0.00004	-0.00234	-2.66488
O	2.57402	-0.68990	0.00065
O	-0.00005	0.00232	2.66487
O	-2.57402	0.68990	-0.00065
O	-1.77485	-1.47634	-1.33118
O	0.79916	-2.16392	1.33437
O	1.77485	1.47635	1.33119
O	-0.79916	2.16393	-1.33436
O	2.76095	-0.73746	2.85915
O	-2.76096	0.73751	-2.85913
O	1.04654	3.90464	-0.00343
O	-1.04653	-3.90464	0.00344
O	2.76108	-0.74251	-2.85778
O	-2.76108	0.74252	2.85778

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/30°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353

C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648

C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556

C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729

C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851

C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465

H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00000	-0.00000	-0.00001
W	1.42452	-0.82418	-1.64496
W	-1.42453	0.82417	1.64495
W	1.42520	-0.82137	1.64574
W	-1.42519	0.82138	-1.64574
W	-1.16358	-2.01504	0.00197
W	1.16359	2.01504	-0.00197
O	2.09589	0.96438	-1.33370
O	-0.21131	2.29923	1.33052
O	-2.09589	-0.96439	1.33370
O	0.21131	-2.29924	-1.33053
O	-0.00057	-0.00227	-2.66488
O	2.30775	-1.33260	0.00065
O	0.00055	0.00225	2.66487
O	-2.30776	1.33260	-0.00065
O	-2.09648	-0.96667	-1.33118
O	0.21186	-2.29703	1.33437
O	2.09649	0.96668	1.33119
O	-0.21186	2.29703	-1.33436
O	2.47601	-1.42692	2.85915
O	-2.47600	1.42697	-2.85913
O	2.02148	3.50073	-0.00343
O	-2.02147	-3.50073	0.00344
O	2.47482	-1.43183	-2.85778
O	-2.47482	1.43184	2.85778

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/45°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809

C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198

C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051

C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799

C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192

H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00000	-0.00000	-0.00001
W	1.16267	-1.16479	-1.64496
W	-1.16268	1.16479	1.64495
W	1.16405	-1.16225	1.64574

W	-1.16404	1.16225	-1.64574
W	-1.64546	-1.64522	0.00197
W	1.64547	1.64522	-0.00197
O	2.27408	0.38907	-1.33370
O	0.39098	2.27558	1.33052
O	-2.27408	-0.38907	1.33370
O	-0.39098	-2.27559	-1.33053
O	-0.00113	-0.00205	-2.66488
O	1.88422	-1.88448	0.00065
O	0.00112	0.00203	2.66487
O	-1.88422	1.88448	-0.00065
O	-2.27524	-0.39112	-1.33118
O	-0.38987	-2.27359	1.33437
O	2.27525	0.39113	1.33119
O	0.38987	2.27359	-1.33436
O	2.02233	-2.01914	2.85915
O	-2.02231	2.01919	-2.85913
O	2.85865	2.85825	-0.00343
O	-2.85864	-2.85825	0.00344
O	2.01991	-2.02358	-2.85778
O	-2.01991	2.02358	2.85778

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/60°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760

C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033

C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612

C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076

C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258

C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156

H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00001	-0.00000	-0.00001
W	0.82077	-1.43203	-1.64013
W	-0.82078	1.43203	1.64013
W	0.82262	-1.41892	1.65054
W	-0.82261	1.41892	-1.65054
W	-2.01593	-1.16202	0.00577
W	2.01593	1.16202	-0.00577
O	2.29722	-0.21866	-1.33287
O	0.96786	2.10069	1.32354
O	-2.29722	0.21866	1.33287
O	-0.96787	-2.10070	-1.32355
O	-0.00151	-0.01061	-2.66486
O	1.33084	-2.30875	0.00844
O	0.00149	0.01060	2.66485
O	-1.33085	2.30875	-0.00844
O	-2.29875	0.20805	-1.33199
O	-0.96639	-2.09014	1.34133
O	2.29876	-0.20804	1.33200
O	0.96640	2.09014	-1.34132

O	1.42916	-2.46505	2.86749
O	-1.42913	2.46510	-2.86746
O	3.50227	2.01878	-0.01003
O	-3.50226	-2.01880	0.01004
O	1.42593	-2.48786	-2.84940
O	-1.42593	2.48786	2.84940

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/75°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508
C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978

C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532
C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094

C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101
C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190

C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364
C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575

C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368
C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464

C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099
H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862

H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00001	-0.00000	-0.00001
W	0.41672	-1.59710	-1.64013
W	-0.41673	1.59710	1.64012
W	0.42199	-1.58491	1.65054
W	-0.42198	1.58491	-1.65054
W	-2.25002	-0.59303	0.00580
W	2.25002	0.59302	-0.00580
O	2.15958	-0.81312	-1.33290
O	1.48463	1.77359	1.32351
O	-2.15958	0.81312	1.33290
O	-1.48464	-1.77359	-1.32351
O	-0.00427	-0.00986	-2.66486
O	0.67920	-2.57685	0.00844
O	0.00425	0.00985	2.66485
O	-0.67920	2.57685	-0.00844
O	-2.16388	0.80327	-1.33196
O	-1.48041	-1.76377	1.34137
O	2.16389	-0.80326	1.33197
O	1.48041	1.76377	-1.34135
O	0.73316	-2.75344	2.86749
O	-0.73312	2.75348	-2.86747
O	3.90896	1.03027	-0.01010
O	-3.90895	-1.03028	0.01010
O	0.72398	-2.77463	-2.84940
O	-0.72398	2.77464	2.84940

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/90°)

241

C	-4.29132	2.48341	-5.68987
C	-1.83417	2.43659	-5.59608
C	0.61785	2.42441	-5.60623
C	3.08069	2.41775	-5.62251
C	5.48963	2.52965	-5.78889
C	-4.28510	3.73369	-4.96508

C	-1.82847	3.65720	-4.88914
C	0.62379	3.65361	-4.89464
C	3.08707	3.65257	-4.90772
C	5.49597	3.72268	-5.09864
C	-5.46769	4.40407	-4.55663
C	-3.06027	4.22098	-4.44637
C	-0.59702	4.20080	-4.43760
C	1.85505	4.18835	-4.43214
C	4.31278	4.24382	-4.51231
C	-5.46300	5.28943	-3.50005
C	-3.05532	5.13630	-3.35167
C	-0.59212	5.11179	-3.34773
C	1.86004	5.09380	-3.35052
C	4.31804	5.17084	-3.40353
C	-4.27528	5.56754	-2.77370
C	-1.81835	5.46587	-2.72551
C	0.63354	5.45978	-2.73551
C	3.09714	5.46184	-2.74610
C	5.50633	5.65189	-2.79347
C	-4.27173	6.05926	-1.41462
C	-1.81499	5.94658	-1.39932
C	0.63650	5.94255	-1.39978
C	3.10006	5.94809	-1.40495
C	5.50857	6.12437	-1.49866
C	-5.45551	6.31290	-0.67327
C	-3.04836	6.09596	-0.70095
C	-0.58537	6.06975	-0.70057
C	1.86640	6.05311	-0.69913
C	4.32328	6.14703	-0.71809
C	-5.45383	6.31205	0.70546
C	-3.04673	6.09429	0.72602
C	-0.58404	6.06760	0.71986
C	1.86797	6.05078	0.71156
C	4.32477	6.14317	0.72691
C	-4.26812	6.05605	1.44334
C	-1.81218	5.94263	1.42151
C	0.63978	5.93849	1.41532

C	3.10282	5.94243	1.41461
C	5.51124	6.11828	1.50568
C	-4.26865	5.56028	2.80107
C	-1.81279	5.45845	2.74660
C	0.63910	5.45065	2.74936
C	3.10225	5.45165	2.75421
C	5.51069	5.64481	2.80033
C	-5.45530	5.28061	3.52855
C	-3.04824	5.12674	3.37500
C	-0.58515	5.10156	3.36399
C	1.86652	5.08155	3.35996
C	4.32381	5.16078	3.41022
C	-5.45844	4.39243	4.58278
C	-3.05137	4.20767	4.46648
C	-0.58811	4.18665	4.45063
C	1.86342	4.17286	4.43861
C	4.32091	4.23055	4.51653
C	-4.27543	3.71963	4.98698
C	-1.81861	3.64205	4.90410
C	0.63317	3.63695	4.90258
C	3.09638	3.63642	4.91099
C	5.50466	3.70901	5.10094
C	-4.28014	2.46622	5.70710
C	-1.82343	2.41920	5.60742
C	0.62823	2.40571	5.61059
C	3.09147	2.39976	5.62240
C	5.49964	2.51404	5.78827
C	-5.46854	1.78583	6.08110
C	-3.06084	1.76351	5.87198
C	-0.59786	1.74623	5.85431
C	1.85404	1.72899	5.84525
C	4.31097	1.75314	5.94132
C	-5.47456	0.42824	6.31990
C	-3.06693	0.35783	6.11750
C	-0.60398	0.34727	6.09960
C	1.84807	0.33997	6.08914
C	4.30486	0.32950	6.19101

C	-4.29231	-0.34835	6.20020
C	-1.83558	-0.35938	6.09345
C	0.61635	-0.36593	6.09703
C	3.07953	-0.37696	6.10966
C	5.48690	-0.44798	6.30634
C	-4.29897	-1.77147	5.94731
C	-1.84223	-1.74791	5.84612
C	0.60964	-1.76414	5.84805
C	3.07279	-1.78151	5.85970
C	5.48066	-1.80496	6.06446
C	-5.48840	-2.53098	5.79371
C	-3.08022	-2.41774	5.62426
C	-0.61690	-2.42372	5.60635
C	1.83473	-2.43592	5.59556
C	4.29164	-2.48381	5.68966
C	-5.49440	-3.72334	5.10175
C	-3.08627	-3.65173	4.90825
C	-0.62324	-3.65261	4.89426
C	1.82845	-3.65593	4.88762
C	4.28519	-3.73435	4.96500
C	-4.31162	-4.24325	4.51385
C	-1.85463	-4.18723	4.43190
C	0.59708	-4.19972	4.43624
C	3.06008	-4.22022	4.44470
C	5.46690	-4.40743	4.55807
C	-4.31676	-5.17047	3.40514
C	-1.85974	-5.09198	3.34958
C	0.59154	-5.11078	3.34647
C	3.05444	-5.13591	3.35051
C	5.46123	-5.29316	3.50146
C	-5.50520	-5.65229	2.79619
C	-3.09669	-5.46006	2.74528
C	-0.63387	-5.45834	2.73421
C	1.81744	-5.46562	2.72458
C	4.27398	-5.56916	2.77381
C	-5.50869	-6.12078	1.49956
C	-3.10040	-5.94590	1.40364

C	-0.63751	-5.94205	1.39880
C	1.81412	-5.94643	1.39865
C	4.27068	-6.06137	1.41490
C	-4.32423	-6.14300	0.71776
C	-1.86700	-6.05246	0.69761
C	0.58446	-6.07014	0.70006
C	3.04757	-6.09679	0.70076
C	5.45441	-6.31581	0.67380
C	-4.32587	-6.14124	-0.72756
C	-1.86866	-6.05094	-0.71308
C	0.58286	-6.06759	-0.72027
C	3.04590	-6.09396	-0.72606
C	5.45281	-6.31353	-0.70485
C	-5.51212	-6.11785	-1.50729
C	-3.10349	-5.94230	-1.41570
C	-0.64045	-5.93843	-1.41647
C	1.81124	-5.94102	-1.42094
C	4.26756	-6.05651	-1.44277
C	-5.51097	-5.64569	-2.80249
C	-3.10244	-5.45273	-2.75562
C	-0.63931	-5.45082	-2.75027
C	1.81232	-5.45704	-2.74575
C	4.26839	-5.56072	-2.80042
C	-4.32380	-5.16204	-3.41226
C	-1.86671	-5.08289	-3.36122
C	0.58507	-5.10096	-3.36432
C	3.04791	-5.12605	-3.37379
C	5.45440	-5.28195	-3.52892
C	-4.32050	-4.23109	-4.51799
C	-1.86350	-4.17396	-4.43973
C	0.58824	-4.18658	-4.45091
C	3.05121	-4.20689	-4.46511
C	5.45792	-4.39251	-4.58226
C	-5.50393	-3.70963	-5.10362
C	-3.09598	-3.63701	-4.91184
C	-0.63319	-3.63788	-4.90319
C	1.81874	-3.64181	-4.90368

C	4.27516	-3.71893	-4.98563
C	-5.49876	-2.51453	-5.79071
C	-3.09087	-2.40008	-5.62312
C	-0.62808	-2.40662	-5.61148
C	1.82366	-2.41923	-5.60747
C	4.28023	-2.46615	-5.70627
C	-4.31007	-1.75338	-5.94258
C	-1.85357	-1.72897	-5.84567
C	0.59809	-1.74653	-5.85457
C	3.06105	-1.76360	-5.87179
C	5.46896	-1.78592	-6.07961
C	-4.30371	-0.32956	-6.19146
C	-1.84724	-0.33968	-6.08877
C	0.60446	-0.34725	-6.09851
C	3.06737	-0.35804	-6.11673
C	5.47504	-0.42824	-6.31711
C	-5.48630	0.44731	-6.30700
C	-3.07864	0.37718	-6.10914
C	-0.61561	0.36645	-6.09608
C	1.83607	0.35887	-6.09208
C	4.29282	0.34859	-6.19788
C	-5.48016	1.80435	-6.06464
C	-3.07226	1.78189	-5.85951
C	-0.60898	1.76491	-5.84797
C	1.84288	1.74783	-5.84566
C	4.29968	1.77121	-5.94368
H	6.43378	2.14599	-6.15735
H	6.44491	4.22547	-4.95380
H	-6.41525	4.17923	-5.03192
H	-6.40700	5.72215	-3.19027
H	6.45239	5.59405	-3.31878
H	6.45623	6.41673	-1.06191
H	-6.40154	6.44787	-1.18427
H	-6.39870	6.44679	1.21864
H	6.45832	6.41154	1.06820
H	6.45714	5.58655	3.32488
H	-6.39965	5.71434	3.22099

H	-6.40540	4.16666	5.05893
H	6.45307	4.21320	4.95713
H	6.44435	2.13064	6.15544
H	-6.41237	2.31683	6.12027
H	-6.42288	-0.04968	6.53567
H	6.43531	0.02888	6.52392
H	6.42448	-2.33608	6.10156
H	-6.43272	-2.14844	6.16287
H	-6.44306	-4.22691	4.95751
H	6.41457	-4.18414	5.03379
H	6.40461	-5.72739	3.19205
H	-6.45063	-5.59547	3.32273
H	-6.45674	-6.41258	1.06331
H	6.40037	-6.45188	1.18465
H	6.39766	-6.44816	-1.21817
H	-6.45933	-6.41124	-1.07022
H	-6.45722	-5.58827	-3.32756
H	6.39867	-5.71643	-3.22224
H	6.40477	-4.16667	-5.05857
H	-6.45225	-4.21444	-4.96142
H	-6.44326	-2.13145	-6.15878
H	6.41270	-2.31728	-6.11862
H	6.42345	0.04971	-6.53266
H	-6.43461	-0.02997	-6.52429
H	-6.42391	2.33561	-6.10138
O	-0.00001	0.00000	-0.00001
W	-0.01084	-1.65053	-1.64013
W	0.01083	1.65054	1.64012
W	-0.00260	-1.64013	1.65054
W	0.00261	1.64012	-1.65054
W	-2.32684	0.00953	0.00580
W	2.32684	-0.00954	-0.00580
O	1.87554	-1.34435	-1.33290
O	1.89308	1.32890	1.32351
O	-1.87555	1.34435	1.33290
O	-1.89309	-1.32891	-1.32351
O	-0.00668	-0.00841	-2.66486

O	-0.01089	-2.66484	0.00844
O	0.00666	0.00842	2.66485
O	0.01088	2.66484	-0.00844
O	-1.88225	1.33595	-1.33196
O	-1.88646	-1.32051	1.34137
O	1.88226	-1.33595	1.33197
O	1.88647	1.32051	-1.34135
O	-0.00447	-2.84938	2.86749
O	0.00452	2.84940	-2.86747
O	4.04242	-0.01655	-0.01010
O	-4.04241	0.01653	0.01010
O	-0.01882	-2.86747	-2.84940
O	0.01882	2.86747	2.84940

W₆O₁₉²⁻@(9,9) h-CNT (y/z = 45°/36°)

241

C	-4.437601	3.163085	-4.843956
C	-1.971838	3.150210	-4.775550
C	0.488927	3.147617	-4.754218
C	2.959625	3.182878	-4.788170
C	5.374943	3.337086	-4.930682
C	-4.445270	4.332086	-3.998180
C	-1.979435	4.286213	-3.941282
C	0.481458	4.285301	-3.911711
C	2.952378	4.325100	-3.933853
C	5.368043	4.437168	-4.104607
C	-5.642150	4.917767	-3.503224
C	-3.220655	4.777483	-3.436090
C	-0.751211	4.767049	-3.410181
C	1.710904	4.779003	-3.394943
C	4.174227	4.884387	-3.476685
C	-5.647693	5.667508	-2.350164
C	-3.227067	5.548427	-2.235521
C	-0.755143	5.537067	-2.220935
C	1.705638	5.561591	-2.224561
C	4.168139	5.690846	-2.278714
C	-4.455786	5.886175	-1.607517

C	-1.990300	5.806244	-1.570625
C	0.470154	5.831346	-1.575533
C	2.941308	5.898137	-1.594044
C	5.358262	6.107231	-1.623677
C	-4.456711	6.213150	-0.200129
C	-1.990786	6.130791	-0.199900
C	0.470745	6.178494	-0.202060
C	2.939784	6.256904	-0.213818
C	5.357637	6.442646	-0.289908
C	-5.647024	6.342390	0.565555
C	-3.227823	6.192297	0.510565
C	-0.756387	6.196760	0.503353
C	1.703743	6.265253	0.500305
C	4.167014	6.392558	0.484661
C	-5.639356	6.199418	1.934003
C	-3.219941	6.042178	1.929769
C	-0.748541	6.044257	1.910918
C	1.711609	6.107192	1.900138
C	4.175088	6.230343	1.918381
C	-4.440825	5.915249	2.643181
C	-1.975532	5.831574	2.597497
C	0.485854	5.872686	2.581299
C	2.954950	5.943159	2.582174
C	5.373637	6.108649	2.672534
C	-4.425837	5.300052	3.950339
C	-1.962139	5.221322	3.866368
C	0.498139	5.239805	3.848348
C	2.969649	5.295050	3.852357
C	5.387461	5.489066	3.900285
C	-5.609818	4.933304	4.646501
C	-3.192512	4.830061	4.474686
C	-0.721439	4.816639	4.429615
C	1.739074	4.833859	4.409744
C	4.202637	4.943495	4.463018
C	-5.596203	3.948631	5.606960
C	-3.177365	3.817387	5.479640
C	-0.708407	3.807982	5.424365

C	1.753457	3.817637	5.383732
C	4.217946	3.897184	5.458233
C	-4.397913	3.262178	5.944647
C	-1.933178	3.224669	5.850448
C	0.527304	3.225889	5.794655
C	2.998504	3.254774	5.797192
C	5.416597	3.321362	5.959282
C	-4.387316	1.933948	6.509478
C	-1.922106	1.932316	6.411911
C	0.538640	1.931329	6.366927
C	3.009625	1.954368	6.383888
C	5.426988	2.069696	6.530254
C	-5.574672	1.194878	6.764960
C	-3.154837	1.235245	6.592137
C	-0.685549	1.244355	6.547601
C	1.776083	1.250584	6.529731
C	4.240317	1.294931	6.639369
C	-5.564958	-0.179917	6.818441
C	-3.145625	-0.190682	6.642542
C	-0.674213	-0.170524	6.616399
C	1.785761	-0.153057	6.633097
C	4.248432	-0.143608	6.766049
C	-4.366184	-0.917540	6.620486
C	-1.901911	-0.880742	6.523365
C	0.558006	-0.863411	6.546365
C	3.028687	-0.853961	6.610707
C	5.445643	-0.907997	6.810581
C	-4.353082	-2.296794	6.187938
C	-1.888287	-2.228129	6.113540
C	0.572993	-2.225381	6.158472
C	3.041599	-2.228796	6.232933
C	5.458483	-2.232891	6.442027
C	-5.535302	-3.036802	5.914319
C	-3.118167	-2.886344	5.809149
C	-0.647392	-2.856462	5.818338
C	1.812624	-2.863375	5.881097
C	4.275956	-2.888812	6.003408

C	-5.515014	-4.150487	5.105959
C	-3.097193	-4.039262	4.968145
C	-0.626993	-3.996471	4.979344
C	1.832662	-3.995159	5.042789
C	4.297238	-4.041735	5.136628
C	-4.311454	-4.611226	4.506094
C	-1.847975	-4.497517	4.450726
C	0.612513	-4.476780	4.494984
C	3.081819	-4.482210	4.552982
C	5.502781	-4.609527	4.642051
C	-4.287003	-5.448355	3.328719
C	-1.825772	-5.296037	3.291068
C	0.633052	-5.247981	3.307298
C	3.104245	-5.236464	3.343253
C	5.524125	-5.338723	3.476268
C	-5.466432	-5.899339	2.676704
C	-3.052512	-5.656334	2.657143
C	-0.583084	-5.561530	2.654715
C	1.875706	-5.500247	2.666438
C	4.340354	-5.553768	2.720658
C	-5.452656	-6.264522	1.350692
C	-3.036624	-6.042729	1.283979
C	-0.570046	-5.922730	1.285005
C	1.888706	-5.818528	1.295160
C	4.354916	-5.856628	1.308535
C	-4.258428	-6.208690	0.581258
C	-1.796566	-6.041338	0.576615
C	0.660341	-5.912865	0.586022
C	3.130042	-5.850985	0.591267
C	5.552013	-5.949841	0.548638
C	-4.261544	-6.058593	-0.853818
C	-1.800151	-5.888556	-0.824582
C	0.657081	-5.761361	-0.821659
C	3.126349	-5.697652	-0.826902
C	5.548399	-5.799159	-0.818950
C	-5.458532	-5.960777	-1.614841
C	-3.043425	-5.744230	-1.510830

C	-0.577258	-5.622093	-1.499105
C	1.881514	-5.516512	-1.501376
C	4.347243	-5.545613	-1.534214
C	-5.480046	-5.325381	-2.834462
C	-3.066931	-5.080825	-2.773807
C	-0.597853	-4.980162	-2.762071
C	1.860802	-4.911039	-2.772102
C	4.325099	-4.940393	-2.845164
C	-4.305276	-4.740601	-3.380950
C	-1.844179	-4.589471	-3.322183
C	0.614345	-4.530600	-3.338366
C	3.085129	-4.501993	-3.380643
C	5.505869	-4.557070	-3.535921
C	-4.338680	-3.665858	-4.345885
C	-1.874739	-3.557896	-4.280633
C	0.585719	-3.519651	-4.330252
C	3.055022	-3.503585	-4.398227
C	5.477538	-3.591330	-4.514642
C	-5.547533	-3.086564	-4.818413
C	-3.128472	-3.000365	-4.675885
C	-0.657905	-2.948088	-4.691287
C	1.801986	-2.924740	-4.763879
C	4.266523	-2.939639	-4.874132
C	-5.575660	-1.818389	-5.352212
C	-3.157171	-1.688098	-5.236450
C	-0.686096	-1.649725	-5.256064
C	1.774019	-1.635282	-5.330501
C	4.237066	-1.625498	-5.468035
C	-4.396250	-1.032578	-5.462157
C	-1.930377	-0.975004	-5.396181
C	0.530801	-0.955388	-5.454619
C	2.999706	-0.935276	-5.541170
C	5.415230	-0.886132	-5.760956
C	-4.414672	0.407613	-5.577016
C	-1.949237	0.429543	-5.500464
C	0.510599	0.458580	-5.536294
C	2.981633	0.488599	-5.612999

C	5.397166	0.486826	-5.835968
C	-5.616881	1.165105	-5.592566
C	-3.194801	1.125344	-5.454303
C	-0.723265	1.147042	-5.446756
C	1.737001	1.174212	-5.475831
C	4.198977	1.219926	-5.621069
C	-5.627082	2.494576	-5.241795
C	-3.205107	2.505417	-5.092809
C	-0.735918	2.513086	-5.071318
C	1.725859	2.522596	-5.071321
C	4.188868	2.598634	-5.191023
H	6.328788	2.978042	-5.305399
H	6.316497	4.905522	-3.859313
H	-6.591664	4.696996	-3.982237
H	-6.600710	6.013979	-1.960786
H	6.307998	6.069980	-2.149225
H	6.307883	6.656371	0.190604
H	-6.602621	6.461553	0.063397
H	-6.589244	6.209889	2.460401
H	6.319427	6.422459	2.240758
H	6.342238	5.337156	4.395159
H	-6.564099	5.363054	4.356002
H	-6.541279	3.632727	6.039355
H	6.364658	3.829320	5.809299
H	6.383163	1.636868	6.809288
H	-6.529810	1.708617	6.823555
H	-6.511622	-0.702340	6.921780
H	6.389224	-0.424187	7.045311
H	6.413045	-2.749298	6.396789
H	-6.495560	-2.671679	6.266539
H	-6.460117	-4.621560	4.852581
H	6.446783	-4.387833	5.131322
H	6.482861	-5.670091	3.088015
H	-6.418886	-5.869465	3.197934
H	-6.396203	-6.504876	0.869428
H	6.507395	-6.051298	1.054524
H	6.501063	-5.786484	-1.339870

H	-6.399077	-6.299512	-1.189969
H	-6.435387	-5.188915	-3.333079
H	6.467679	-4.956004	-3.227636
H	6.419455	-3.258987	-4.941125
H	-6.489158	-3.609086	-4.677229
H	-6.538160	-1.388850	-5.614196
H	6.371158	-1.396854	-5.833010
H	6.337812	1.012875	-5.970768
H	-6.565146	0.673470	-5.790683
H	-6.583643	3.004013	-5.171979
O	0.130983	0.108060	0.547227
W	1.502243	-0.694479	-1.219347
W	-1.245008	0.913567	2.314752
W	1.516370	-0.989989	2.134284
W	-1.257594	1.209539	-1.041296
W	-1.216900	-1.842719	0.380144
W	1.475526	2.062768	0.714566
O	2.297706	1.026908	-0.730961
O	0.108400	2.326068	2.103771
O	-2.037917	-0.808293	1.826116
O	0.149946	-2.108132	-1.011184
O	0.115688	0.346150	-2.152157
O	2.331331	-1.413756	0.402710
O	0.141068	-0.129465	3.245483
O	-2.070576	1.629012	0.691202
O	-2.051203	-0.570310	-0.851766
O	0.163048	-2.348668	1.688867
O	2.310753	0.789503	1.946494
O	0.097355	2.564802	-0.595244
O	2.547822	-1.781735	3.288960
O	-2.291434	2.006748	-2.189373
O	2.476321	3.478906	0.839574
O	-2.224804	-3.254158	0.257502
O	2.522793	-1.272210	-2.502661
O	-2.270777	1.494560	3.592840

W₆O₁₉²⁻@(10,10) h-CNT

265

C	-4.299003	2.117629	-6.532245
C	-1.842395	2.091898	-6.428294
C	0.610347	2.089968	-6.431590
C	3.073043	2.100992	-6.463069
C	5.482319	2.203208	-6.626341
C	-4.300355	3.437880	-5.945780
C	-1.843461	3.382358	-5.857820
C	0.609434	3.388125	-5.856641
C	3.072209	3.405650	-5.883964
C	5.481637	3.459853	-6.067828
C	-5.488438	4.134862	-5.612523
C	-3.078240	3.994584	-5.494296
C	-0.615070	3.981330	-5.472989
C	1.837907	3.986786	-5.472079
C	4.294179	4.047052	-5.564474
C	-5.488926	5.157649	-4.693344
C	-3.078653	5.056921	-4.540912
C	-0.615510	5.039052	-4.525850
C	1.837501	5.037984	-4.531163
C	4.293965	5.122277	-4.600021
C	-4.301246	5.564439	-4.036030
C	-1.844237	5.486519	-3.972533
C	0.608872	5.486457	-3.978684
C	3.071791	5.510627	-3.997980
C	5.481251	5.686084	-4.070212
C	-4.300754	6.289906	-2.787244
C	-1.843644	6.194908	-2.752324
C	0.609477	6.200122	-2.751167
C	3.072405	6.227579	-2.763812
C	5.481836	6.375803	-2.880784
C	-5.487942	6.659386	-2.107505
C	-3.077566	6.476252	-2.097028
C	-0.614268	6.454046	-2.090526
C	1.838746	6.457650	-2.088671
C	4.295022	6.556985	-2.128764
C	-5.486633	6.949264	-0.763419

C	-3.076111	6.777351	-0.701889
C	-0.612900	6.752902	-0.702490
C	1.840100	6.753091	-0.709213
C	4.296602	6.858094	-0.716553
C	-4.297787	6.893401	0.005707
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C	-3.072391	6.487940	2.108229
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