

# Supporting Information

## Calibrations on the basic strength of the nitrogen groups on the nanostructured carbon materials

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## Computational Setup

The most calculations except Fukui Functions part are carried out by using Gaussian09 program.<sup>1</sup> The structure optimization and frequency analysis are performed at the PBE/3-21G level. Further, the energy is refined at the B3LYP/6-31G(d) level. The gas phase Gibbs free energy is taken as the sum of the electronic energy computed at B3LYP/6-31G(d) and the thermal corrections computed at PBE/3-21G. This methodology has been exercised before for the basicity calculations.<sup>2</sup> The Gibbs free energy calculation in water is carried out at the same level of theory with the gas phase and adopted the gas phase structure. The solvent, which is the water, is represented as polarizable continuum model (PCM) using the integral equation formalism. The Fukui Functions calculations setup is described in our previous work.<sup>3</sup>

## References

- (1) Frisch, M. J. et al. *Gaussian09 Revision D.01*, Gaussian Inc. Wallingford CT 2009.
- (2) Menéndez, J. A.; Suárez, D.; Fuente, E.; Montes-Morán, M. A. *Carbon* **1999**, *37*, 1002 – 1006.
- (3) Li, B.; Su, D. *Chem. Eur. J.* **2014**, *20*, 7890–7894.

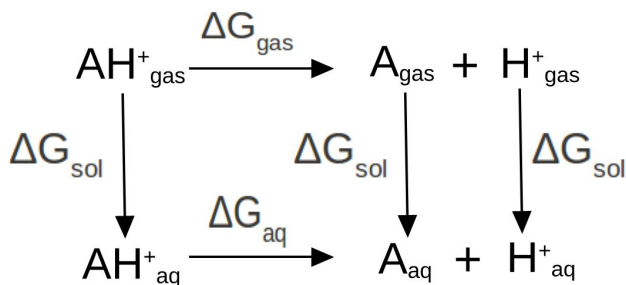


Figure S1: The thermodynamic cycle indicates that the procedure leads to the equation 2 in order to calculate  $pK_a$ .

**Table S1: The contributions percentage (%) from the  $p$  orbital of the nitrogen group for the bonding orbital between the nitrogen and carbon on the graphene and carbon nanotubes.**

groups	graphene	(5,5)	(9,0)	(11,0)
N0	64.87	65.35	65.92	65.87
N1	66.68	66.92	67.54	67.0
N2	63.58	64.50	64.40	64.24
N3	69.15	69.70		

**Table S2: The charges for the nitrogen atom on graphene and SWCNTs from the NBO analysis.**

groups	graphene	(5,5)	(9,0)	(11,0)
N0	-0.45	-0.45	-0.52	-0.49
N1	-0.30	-0.30	-0.33	-0.34
N2	-0.35	-0.40	-0.39	-0.39
N3	-0.48	-0.40		

**Table S3: The proton affinity (PA, kcal/mol) at the graphitic nitrogen site on the graphene calculated with B3LYP functional by using three different basis sets.**

basis set	6-31G(d)	6-31+G(d)	6-311G(d)
PA (kcal/mol)	208.7	203.4	203.5

## The coordinates of N0 group on graphene

N -7.20256700 -6.16196500 -0.00002000  
C -7.84272700 -4.98130500 -0.00002400  
C -7.18112200 -3.71679700 -0.00001600  
C -5.73893700 -3.72165700 -0.00001500  
C -5.05156900 -4.97233700 -0.00001900  
C -5.83785300 -6.14658800 -0.00001700  
C -5.02171700 -2.48128600 -0.00001100  
C -5.73603100 -1.25302900 -0.00000600  
C -7.19257900 -1.25710500 -0.00000600  
C -7.87922300 -2.49224800 -0.00001000  
C -5.02538100 -0.01156000 -0.00000200  
C -5.74291700 1.22519100 0.00000400  
C -7.19781100 1.21320200 0.00000400  
C -7.88123000 -0.02378100 -0.00000100  
C -5.04092000 2.46234800 0.00001000  
C -5.76853000 3.70136800 0.00001600  
C -7.21653300 3.67940800 0.00001200  
C -7.89384700 2.44035900 0.00000700  
C -5.07947100 4.95523800 0.00002400  
C -5.83856700 6.14768100 0.00001400  
C -7.24578400 6.12232100 0.00000900  
C -7.93161900 4.91298800 0.00001000  
C -3.60011900 2.46724500 0.00000500  
C -2.89234500 3.71890200 0.00001400  
C -3.61399000 4.95736300 0.00003700

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C -0.74263700 4.96361400 0.00001300  
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C -2.87544300 6.16214800 0.00008100  
C -0.72691400 2.47644700 -0.00000600  
C 0.71237100 2.47961000 -0.00000400  
C 1.43093300 3.72823600 -0.00001400  
C 0.71574000 4.96693600 -0.00002600  
C 2.87127500 3.73191000 -0.00001900  
C 3.58679800 4.97388300 -0.00004000  
C 2.84267200 6.17521800 -0.00009200  
C 1.45631900 6.17255800 -0.00008600  
C 3.58488700 2.48351400 -0.00000900  
C 5.02542700 2.48527700 -0.00001100  
C 5.74726500 3.72813400 -0.00001200  
C 5.05222600 4.97873700 -0.00001800  
C 7.19545500 3.71417200 -0.00000100  
C 7.90463700 4.95117500 0.00001000  
C 7.21276900 6.15693100 0.00001500  
C 5.80547200 6.17492700 0.00000300  
C -2.87990800 1.23646400 -0.00000200  
C -1.43636200 1.23949400 -0.00000500  
C 1.42815200 1.24587200 -0.00000300  
C 2.87132900 1.24897000 -0.00000400  
C 5.73280800 1.25118500 -0.00000500  
C 7.18758800 1.24877100 -0.00000100  
C 7.87847200 2.47866500 0.00000200

C -3.58911800 -0.00869500 -0.00000400  
C -0.71772300 -0.00220400 -0.00000400  
C 0.71649400 0.00056000 -0.00000300  
C 3.58624600 0.00657600 -0.00000200  
C 5.02172800 0.00965800 -0.00000100  
C -2.87126600 -1.24949700 -0.00000500  
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C -3.58956800 -4.97512600 -0.00001900  
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C 7.23992700 -6.12781800 -0.00000600  
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H -3.37293600 -7.13660800 -0.00004700  
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H 0.96986200 -7.13112200 0.00009600  
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H 0.93831600 7.13173300 -0.00014100  
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H 7.76032000 7.10247800 0.00003100

**the coordiantes of N1 group on graphene**

C 7.20540000 -6.14986200 0.00150800  
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C 1.46306900 -6.15773100 0.00050100  
C -1.46929300 -6.16240700 -0.00145400  
C -2.85442800 -6.16093200 -0.00155600  
C -5.81192200 -6.16571600 -0.00030300  
C -7.21933700 -6.14240200 -0.00017800  
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C -0.72900400 -4.95707900 -0.00065400  
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C -5.06175400 -4.96851500 -0.00058300  
C -7.90869600 -4.93589800 -0.00029300  
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C -5.73303200 1.24128500 -0.00050100  
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C -1.46251900 6.16424800 -0.00056900  
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H -3.36536000 7.12342800 -0.00074900  
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H -9.00171100 -4.91462800 -0.00022300

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H 8.96260400 -0.00581700 0.00139200  
H -8.96815800 0.00615000 -0.00052200  
H 8.97082200 2.45650000 0.00111500  
H -8.97063600 2.46654300 -0.00058700  
H 8.99641900 4.91518500 0.00083900  
H -8.99335700 4.92258400 -0.00064000  
H 7.75477000 -7.09454000 0.00165000  
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**the coordiantes of N2 group on graphene**

C -7.20288700 6.14112300 -0.03519200  
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C 2.86501600 6.18814400 0.11451200  
C 5.83458600 6.17027400 0.03463100  
C 7.23994700 6.13807600 0.00515800

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C 3.60794400 4.98886000 0.05365800  
C 5.06946000 4.98058000 0.02474900  
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C -7.18969400 3.70008300 -0.05902700  
C -5.74275600 3.71145000 -0.02575700  
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C 2.81720500 -1.28122200 -0.07476500  
C 5.69404300 -1.23853000 -0.06918700  
C 7.14830400 -1.23057200 -0.08703600  
C -7.87400100 -2.46309300 -0.08620200  
C -5.02024500 -2.47113700 -0.02148100  
C -3.57881700 -2.46894300 0.01214500  
C -0.68916100 -2.44618200 0.05768800  
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C 7.85556900 -2.44974700 -0.08140900  
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C 2.86500400 -6.18814600 0.11456000  
C 5.83457400 -6.17028000 0.03472500  
C 7.23993500 -6.13808400 0.00526700  
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H -5.29011800 -7.12136000 0.02144800

H -3.36125900 -7.11430000 0.05231900  
H -0.94025000 -7.10754600 0.08713400  
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H -8.98986700 -4.91800500 -0.08851100  
H 9.00998300 -4.89006700 -0.05486900  
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H -0.94024000 7.10754300 0.08737100  
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H 3.38300800 7.14745900 0.14840200  
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H 7.79884200 7.07692400 0.01344300

**the coordiantes of N3 group on graphene**



C -8.01522100 -6.75023200 -0.33925500  
C -5.04169700 -6.82618200 -0.13452700  
C -3.65188900 -6.84823500 -0.04443300  
C -0.67873900 -6.87258400 0.03581300  
C 0.70911400 -6.87008600 0.03681100  
C 3.68241400 -6.83829100 -0.03874800  
C 5.07067100 -6.81098900 -0.12742500  
C 8.04561900 -6.71925300 -0.33160700  
C -7.24294500 -5.59012900 -0.27958500  
C -5.76541200 -5.61697900 -0.15547100  
C -2.89147900 -5.65846100 0.03851700  
C -1.42847200 -5.67026200 0.09015400  
C 1.45513900 -5.66540000 0.09213800  
C 2.91753200 -5.64906700 0.04256100  
C 5.79090400 -5.59778100 -0.14870000  
C 7.26661600 -5.56455000 -0.27189500  
C -7.87940100 -4.32098900 -0.34385700  
C -5.03535900 -4.38663400 -0.06282600  
C -3.59593800 -4.40950400 0.04638000  
C -0.71062100 -4.43587600 0.17434300  
C 0.73266400 -4.43314200 0.17533300  
C 3.61700000 -4.39860800 0.05050600  
C 5.05633400 -4.37019500 -0.05725300  
C 7.89782700 -4.28997400 -0.33576600  
C -7.17034900 -3.09508500 -0.26607000  
C -5.72442000 -3.12482300 -0.09976700  
C -2.86854500 -3.17572300 0.16194200

C -1.43178200 -3.19139600 0.23977500  
C 1.44918100 -3.18669000 0.24132400  
C 2.88478600 -3.16596600 0.16488400  
C 5.74088300 -3.10626100 -0.09426000  
C 7.18418000 -3.07097400 -0.25867700  
C -7.83258000 -1.85568500 -0.35467700  
C -5.00653500 -1.90622300 0.01450300  
C -3.57294700 -1.93225800 0.17243000  
C -0.71511300 -1.96695600 0.36388300  
C 0.72744200 -1.96391000 0.36471300  
C 3.58469900 -1.91968000 0.17564300  
C 5.01826500 -1.88766500 0.01871800  
C 7.84254000 -1.82326600 -0.34734300  
C -7.13319700 -0.62099800 -0.27093400  
C -5.69724300 -0.64801300 -0.05681400  
C -2.85916000 -0.70595500 0.32449100  
C -1.43096900 -0.73051400 0.44388100  
C 1.43779000 -0.72591100 0.44478900  
C 2.86587300 -0.69580600 0.32686100  
C 5.70333200 -0.62910900 -0.05283700  
C 7.13906600 -0.59539400 -0.26546900  
C -7.78964800 0.62305300 -0.40188600  
C -4.98237500 0.57517600 0.06396600  
C -3.56222900 0.54772400 0.29692000  
C -0.71728400 0.49408600 0.60183100  
C 0.71852000 0.49725400 0.60190700  
C 3.56439100 0.56025800 0.29922300

C 4.98223800 0.59407700 0.06700400  
C 7.78997100 0.65611200 -0.39753800  
C -7.08564600 1.85309600 -0.33077700  
C -5.65949800 1.83106700 -0.07568100  
C -2.85498800 1.76854300 0.46118400  
C -1.43365700 1.72507700 0.66021100  
C 1.42897200 1.73038900 0.66000900  
C 2.85096700 1.77995100 0.46192600  
C 5.65298700 1.85312800 -0.07427600  
C 7.07965700 1.88316500 -0.32965900  
C -7.72266100 3.10576800 -0.50458500  
C -4.93900100 3.05703800 0.00824900  
C -3.53958500 3.03296100 0.31764300  
C -0.72034400 2.94119600 0.80301000  
C 0.70987200 2.94446100 0.80290800  
C 3.52915600 3.04359700 0.31779000  
C 4.92517700 3.07527200 0.00848400  
C 7.70718600 3.13888700 -0.50713400  
C -7.00933000 4.32850500 -0.45899700  
C -5.58164200 4.32011300 -0.20336400  
C -2.82140100 4.25206500 0.40429300  
C -1.43780400 4.17671800 0.71819100  
C 1.42101900 4.18263400 0.71819600  
C 2.80309900 4.26441700 0.40176000  
C 5.55982800 4.34537300 -0.20886000  
C 6.98489200 4.36126100 -0.46666600  
C -7.67064600 5.57827400 -0.66477300

C -4.84081500 5.56602600 -0.17997500  
C -3.38364500 5.55216500 0.06571600  
C -0.70561900 5.34759200 0.67752500  
C 0.68244800 5.35133800 0.67868400  
C 3.35722900 5.56065200 0.06009100  
C 4.81076800 5.58392100 -0.19275200  
C 7.63576600 5.61171000 -0.68153900  
C -6.95154900 6.76557600 -0.61803800  
C -5.56064200 6.76176300 -0.37581200  
C -2.54103200 6.69788800 -0.09811500  
C -1.13855000 6.61657800 0.15822900  
C 1.10979500 6.61820500 0.15984100  
C 2.50428000 6.70753600 -0.10299400  
C 5.52003000 6.78703300 -0.40289400  
C 6.90783300 6.79740800 -0.64477100  
H -7.58999500 -7.75261000 -0.28778900  
H -5.57429200 -7.77617600 -0.20126500  
H -3.14980300 -7.81657200 -0.04286800  
H -1.19359600 -7.83247900 -0.02170700  
H 1.22748600 -7.82810200 -0.02000800  
H 3.18316700 -7.80807100 -0.03661700  
H 5.60769100 -7.75868100 -0.19284000  
H 7.62628900 -7.72424300 -0.28104100  
H -7.46318700 7.71990000 -0.76404600  
H -5.03441900 7.71696800 -0.32380400  
H -2.96292400 7.62221900 -0.49885700  
H 2.92093900 7.63114500 -0.51042200

H 4.98560000 7.73794900 -0.36028600  
H 7.41474300 7.75287300 -0.79996000  
H -9.10119200 -6.67721300 -0.43626400  
H 9.13122000 -6.63986300 -0.42797300  
H -8.96754600 -4.28916300 -0.45522500  
H 8.98594000 -4.25422600 -0.44688400  
H -8.91722100 -1.84158100 -0.49899500  
H 8.92720000 -1.80593000 -0.49123400  
H -8.86996900 0.63809700 -0.57656900  
H 8.87019200 0.67595100 -0.57180700  
H -8.80044500 3.13196100 -0.69393900  
H 8.78450300 3.17232900 -0.69785400  
H -8.74739900 5.58130100 -0.85405500  
H 8.71231900 5.62178900 -0.87205900  
N -0.02334100 7.43313000 -0.13872900

**the coordiantes of N0 group on (5,5) SWCNT**

C -6.18250500 3.38815700 0.98654700  
C -1.24651100 3.32603100 0.92749100  
C -2.49076500 3.43676800 0.20942000  
C -3.73583600 3.32922900 0.91907200  
C -4.96723800 3.26740000 -1.22105100  
C -4.96903000 3.48012700 0.21114400  
C -6.17873400 2.95989100 -1.94227700  
C 3.71533000 3.33610300 0.92483000  
C 2.47122200 3.44028100 0.21289000

C 1.22567700 3.32855300 0.92922300  
C -0.00874600 3.24396000 -1.21075700  
C -0.00999200 3.45887200 0.21717000  
C -1.24394700 2.90921000 -1.85313100  
C -2.48935500 3.22419700 -1.20061400  
C -3.73209400 1.89783300 -2.88002400  
C -3.73280400 2.91533900 -1.85101700  
C -4.96662800 1.27173600 -3.23600500  
C -6.17788200 1.99130200 -2.92090200  
C 6.16186800 3.40046600 0.99734100  
C 4.95123600 3.27177800 -1.21303100  
C 4.94995600 3.48700600 0.21903800  
C 3.71758500 2.92127300 -1.84591800  
C 2.47238400 3.22793700 -1.19717100  
C 1.22950000 1.90755700 -2.87322100  
C 1.22801700 2.91225900 -1.85181000  
C -0.00583800 1.26872700 -3.21711000  
C -1.24301000 1.90247300 -2.87276000  
C -2.48697900 -0.15462500 -3.43177700  
C -2.48745200 1.25218400 -3.19744600  
C -3.73225400 -0.86826300 -3.33157600  
C -4.97107700 -0.16044200 -3.45673600  
C -6.18449100 -2.14132500 -2.68803900  
C -6.19045600 -0.92401500 -3.33188900  
C 6.16617000 2.00282800 -2.91726600  
C 6.16442400 2.96439000 -1.93121800  
C 4.95514600 1.28928400 -3.24401200

C 3.71941700 1.90993300 -2.88019700  
C 2.47931900 -0.14204200 -3.44079400  
C 2.47604100 1.26357300 -3.20135300  
C 1.23585700 -0.86532300 -3.34439300  
C -0.00352800 -0.15513100 -3.45647800  
C -1.23256200 -2.15730900 -2.70303200  
C -1.23901400 -0.87215000 -3.33781900  
C -2.47468200 -2.67643900 -2.18817100  
C -3.72349200 -2.16198600 -2.68502200  
C -4.94034200 -3.34661500 -0.90178500  
C -4.95456500 -2.67941100 -2.17719600  
N -6.14490900 -3.48929000 -0.22136900  
C 6.17409000 -0.91329400 -3.41747000  
C 4.95882900 -0.13792800 -3.48823000  
C 3.73252600 -2.14571700 -2.70613000  
C 3.72680800 -0.85141500 -3.35230900  
C 2.49017500 -2.65393800 -2.19243200  
C 1.24178800 -2.14860300 -2.70703800  
C 0.01454000 -3.35021000 -0.93034900  
C 0.00803400 -2.67916100 -2.20936000  
C -1.21974400 -3.47434200 -0.21624200  
C -2.46382800 -3.35888800 -0.93368600  
C -3.70849700 -3.25958700 1.20429000  
C -3.70146200 -3.49332700 -0.22050500  
C -4.95047300 -2.95213600 1.83729400  
C -6.13987000 -3.32284300 1.09623000  
C 6.17935700 -2.14513500 -2.80191700

C 4.97344100 -3.34246800 -0.93644600  
C 4.96934700 -2.67639000 -2.22217900  
C 3.73954600 -3.43723800 -0.22012600  
C 2.49475300 -3.31214500 -0.92762600  
C 1.24849300 -3.23717900 1.20246800  
C 1.25080900 -3.44984100 -0.21444500  
C 0.00956000 -2.93233300 1.85364800  
C -1.22303700 -3.25632200 1.20157700  
C -2.48157700 -1.91589000 2.85260700  
C -2.46954800 -2.92755300 1.84731400  
C -3.73149600 -1.28558400 3.18694800  
C -4.96516500 -1.93797900 2.86736000  
C -6.18470200 0.08762000 3.49348800  
C -6.18300900 -1.26843500 3.25195700  
C 6.18507900 -3.30051400 1.19013000  
C 6.18657500 -3.50425400 -0.17207200  
C 4.96995700 -2.92409000 1.87145000  
C 3.73768300 -3.22320500 1.21068800  
C 2.48428100 -1.90035400 2.86653500  
C 2.49096300 -2.89802000 1.84802600  
C 1.23506600 -1.26719500 3.20897000  
C 0.00134600 -1.91722800 2.88070400  
C -1.24409500 0.13886300 3.44023400  
C -1.23873700 -1.27402100 3.20171600  
C -2.49127100 0.85247800 3.32457900  
C -3.73555400 0.13977900 3.43427100  
C -4.97153000 2.15761500 2.72162900



C -4.97130300 0.85653100 3.35791700  
C -6.18373200 2.74667800 2.20534000  
C 6.17280700 -1.23617900 3.31083100  
C 4.96359500 -1.91297600 2.90793700  
C 3.72014700 0.16116800 3.45722000  
C 3.72587600 -1.26507700 3.21443100  
C 2.47320800 0.86650600 3.33673700  
C 1.22945600 0.14583000 3.44710600  
C -0.01071900 2.15387000 2.71174000  
C -0.00900400 0.85985700 3.35205500  
C -1.24715200 2.66051400 2.19650900  
C -2.49236600 2.13086800 2.69276300  
C -3.73685800 2.65416100 2.19871100  
C 6.16732300 0.12123400 3.54274900  
C 4.94974900 2.17880600 2.73790000  
C 4.95214100 0.88399000 3.38607600  
C 3.71506800 2.66824200 2.20814800  
C 2.47095100 2.14270600 2.70085000  
C 1.22527500 2.66547100 2.19945900  
C 6.16182500 2.76663900 2.22017700  
H -7.13156500 2.57011700 2.71882700  
H -7.12930700 3.71075600 0.54744000  
H -7.12501500 3.40351400 -1.62432800  
H -7.12359200 1.67886200 -3.36924100  
H -7.14267500 -0.46585600 -3.60788800  
H -7.11469200 -2.64089300 -2.41071900  
H -7.10387100 -3.40199700 1.60915400

H -7.12990400 -1.81235800 3.22185300  
H -7.13420200 0.60300400 3.65433800  
H 7.13508900 -3.65893000 -0.69133900  
H 7.12818100 -2.66129600 -2.63873200  
H 7.11888400 -0.46674700 -3.73583300  
H 7.11383700 1.68895000 -3.36074400  
H 7.11080500 3.40148000 -1.60471400  
H 7.10908200 3.72231100 0.55851400  
H 7.10889300 2.59406400 2.73642200  
H 7.11185000 0.64111200 3.71836500  
H 7.12172600 -1.77727400 3.30590400  
H 7.13235600 -3.29585700 1.73407400

**the coordiantes of N1 group on (5,5) SWCNT**

C -0.04205100 3.54232400 6.15136300  
C -0.05694500 3.40202200 1.23233700  
C -0.77542200 3.33071400 2.46826500  
C -0.07296500 3.44690800 3.71190800  
C -2.12559900 2.79565000 4.93173000  
C -0.80481300 3.40644400 4.94036700  
C -2.72584400 2.29798500 6.14098900  
C -0.07296500 3.44690800 -3.71190800  
C -0.77542200 3.33071400 -2.46826500  
C -0.05694500 3.40202200 -1.23233700  
C -0.75231900 3.26773000 0.00000000  
C -2.57726700 2.21467900 1.22264200

C -2.07425200 2.73654800 2.45385700  
C -3.31565600 0.99459100 3.71187700  
C -2.61954600 2.26097200 3.70009600  
C -3.48777800 0.30064600 4.94974100  
C -3.38643200 1.08528800 6.15071200  
C -0.04205100 3.54232400 -6.15136300  
C -2.12559900 2.79565000 -4.93173000  
C -0.80481300 3.40644400 -4.94036700  
C -2.61954600 2.26097200 -3.70009600  
C -2.07425200 2.73654800 -2.45385700  
C -3.29932200 0.98111800 -1.22877600  
C -2.57726700 2.21467900 -1.22264200  
C -3.42542200 0.26318300 0.00000000  
C -3.29932200 0.98111800 1.22877600  
C -3.26415300 -1.14012500 2.47650700  
C -3.44138800 0.28065100 2.47256400  
C -2.95821000 -1.78366800 3.72602300  
C -3.30283500 -1.14307100 4.95792400  
C -2.05197800 -2.86193200 6.17038700  
C -2.99874700 -1.85553200 6.16858500  
C -3.38643200 1.08528800 -6.15071200  
C -2.72584400 2.29798500 -6.14098900  
C -3.48777800 0.30064600 -4.94974100  
C -3.31565600 0.99459100 -3.71187700  
C -3.26415300 -1.14012500 -2.47650700  
C -3.44138800 0.28065100 -2.47256400  
C -2.96180900 -1.80688800 -1.24157700

C -3.27534200 -1.16241000 0.00000000  
C -1.97940200 -2.85406500 1.24081600  
C -2.96180900 -1.80688800 1.24157700  
C -1.33622400 -3.18417600 2.48167400  
C -1.96815500 -2.83751000 3.72737300  
C 0.07443400 -3.49030700 4.96216200  
C -1.35324000 -3.21189000 4.96350800  
C 0.85437900 -3.43413600 6.16900600  
C -2.99874700 -1.85553200 -6.16858500  
C -3.30283500 -1.14307100 -4.95792400  
C -1.96815500 -2.83751000 -3.72737300  
C -2.95821000 -1.78366800 -3.72602300  
C -1.33622400 -3.18417600 -2.48167400  
C -1.97940200 -2.85406500 -1.24081600  
C 0.07266100 -3.46114300 0.00000000  
C -1.34486600 -3.19645700 0.00000000  
C 0.78832200 -3.36247500 1.23889300  
C 0.06934600 -3.44614800 2.48035100  
C 2.09184100 -2.74539500 3.72564100  
C 0.78314800 -3.35926700 3.72643100  
C 2.64630100 -2.28476800 4.96086700  
C 2.10503400 -2.84853300 6.16823000  
C -2.05197800 -2.86193200 -6.17038700  
C 0.07443400 -3.49030700 -4.96216200  
C -1.35324000 -3.21189000 -4.96350800  
C 0.78314800 -3.35926700 -3.72643100  
C 0.06934600 -3.44614800 -2.48035100

C 2.08845600 -2.75035800 -1.23835700  
C 0.78832200 -3.36247500 -1.23889300  
C 2.61830300 -2.25956500 0.00000000  
C 2.08845600 -2.75035800 1.23835700  
C 3.30707000 -1.00027500 2.48004500  
C 2.61159200 -2.24920500 2.47921700  
C 3.44889700 -0.29659200 3.72750200  
C 3.34789400 -1.01118100 4.96227500  
C 3.35137800 1.11782200 6.17143700  
C 3.52704200 -0.25222400 6.17081700  
C 2.10503400 -2.84853300 -6.16823000  
C 0.85437900 -3.43413600 -6.16900600  
C 2.64630100 -2.28476800 -4.96086700  
C 2.09184100 -2.74539500 -3.72564100  
C 3.30707000 -1.00027500 -2.48004500  
C 2.61159200 -2.24920500 -2.47921700  
C 3.46148600 -0.29210400 -1.23932600  
C 3.32284400 -1.00025800 0.00000000  
C 3.29037400 1.13497100 1.23979600  
C 3.46148600 -0.29210400 1.23932600  
C 2.96861500 1.78768500 2.47984500  
C 3.26769600 1.13810600 3.72812600  
C 1.98951700 2.86304500 4.95625400  
C 2.99025100 1.80685300 4.96217800  
C 1.31381100 3.27446600 6.15789500  
C 3.52704200 -0.25222400 -6.17081700  
C 3.34789400 -1.01118100 -4.96227500

C 3.26769600 1.13810600 -3.72812600  
C 3.44889700 -0.29659200 -3.72750200  
C 2.96861500 1.78768500 -2.47984500  
C 3.29037400 1.13497100 -1.23979600  
C 2.00144800 2.83391200 0.00000000  
C 2.99780300 1.79222400 0.00000000  
C 1.36475300 3.18001100 1.23293300  
C 1.98638600 2.82747000 2.47694200  
C 1.34976100 3.17736600 3.71824700  
C 3.35137800 1.11782200 -6.17143700  
C 1.98951700 2.86304500 -4.95625400  
C 2.99025100 1.80685300 -4.96217800  
C 1.34976100 3.17736600 -3.71824700  
C 1.98638600 2.82747000 -2.47694200  
C 1.36475300 3.18001100 -1.23293300  
C 1.31381100 3.27446600 -6.15789500  
H 1.84474100 3.24188300 7.11219100  
H -0.55607500 3.71526300 7.09934400  
H -2.53704300 2.81105700 7.08666000  
H -3.70846400 0.65970500 7.10383200  
H -3.41044400 -1.50825400 7.11903500  
H -1.73267800 -3.29115000 7.12281400  
H 0.40241500 -3.72787000 7.11934000  
H 2.62077600 -2.68924700 7.11803000  
H 3.66065700 -0.77351500 7.12151600  
H 3.34973700 1.65574300 7.12234300  
H 0.40241500 -3.72787000 -7.11934000

H -1.73267800 -3.29115000 -7.12281400  
H -3.41044400 -1.50825400 -7.11903500  
H -3.70846400 0.65970500 -7.10383200  
H -2.53704300 2.81105700 -7.08666000  
H -0.55607500 3.71526300 -7.09934400  
H 1.84474100 3.24188300 -7.11219100  
H 3.34973700 1.65574300 -7.12234300  
H 3.66065700 -0.77351500 -7.12151600  
H 2.62077600 -2.68924700 -7.11803000  
N -2.04727200 2.67990400 0.00000000

**the coordiantes of N2 group on (5,5) SWCNT**

C 2.15246100 2.77188700 6.19259900  
C 2.08209000 2.62225600 1.27455500  
C 1.42113100 3.03351800 2.50000200  
C 2.05861700 2.72363600 3.74303100  
C 0.03064100 3.40950900 4.97191500  
C 1.44245600 3.10886200 4.98087300  
C -0.75894300 3.39409800 6.18181000  
C 2.05861700 2.72363600 -3.74303100  
C 1.42113100 3.03351800 -2.50000200  
C 2.08209000 2.62225600 -1.27455500  
C 0.08694200 3.31479100 0.00000000  
C 1.49039100 3.00982900 0.00000000  
C -0.65979100 3.27465700 1.23690400  
C 0.03921400 3.34851800 2.49113000

C -2.02210000 2.77521500 3.72720400  
C -0.68420800 3.31780600 3.73230300  
C -2.59924300 2.33647000 4.96206700  
C -2.03329600 2.87491800 6.17690700  
C 2.15246100 2.77188700 -6.19259900  
C 0.03064100 3.40950900 -4.97191500  
C 1.44245600 3.10886200 -4.98087300  
C -0.68420800 3.31780600 -3.73230300  
C 0.03921400 3.34851800 -2.49113000  
C -1.98885000 2.75439400 -1.23536100  
C -0.65979100 3.27465700 -1.23690400  
C -2.55487400 2.29675600 0.00000000  
C -1.98885000 2.75439400 1.23536100  
C -3.31142500 1.08777800 2.48216400  
C -2.55581400 2.29821800 2.48137700  
C -3.48997400 0.39355400 3.72817300  
C -3.35622800 1.10582500 4.96242900  
C -3.43250000 -1.01326800 6.17961200  
C -3.57418600 0.35550500 6.17735500  
C -2.03329600 2.87491800 -6.17690700  
C -0.75894300 3.39409800 -6.18181000  
C -2.59924300 2.33647000 -4.96206700  
C -2.02210000 2.77521500 -3.72720400  
C -3.31142500 1.08777800 -2.48216400  
C -2.55581400 2.29821800 -2.48137700  
C -3.48639200 0.37971300 -1.23904900  
C -3.32618400 1.08445800 0.00000000



C -3.35555000 -1.04534300 1.23975500  
C -3.48639200 0.37971300 1.23904900  
C -3.04623900 -1.70039000 2.48687000  
C -3.34855700 -1.04584300 3.73085700  
C -2.07396300 -2.76005800 4.96888900  
C -3.06882100 -1.70980000 4.96762400  
C -1.39467900 -3.15476000 6.17988700  
C -3.57418600 0.35550500 -6.17735500  
C -3.35622800 1.10582500 -4.96242900  
C -3.34855700 -1.04584300 -3.73085700  
C -3.48997400 0.39355400 -3.72817300  
C -3.04623900 -1.70039000 -2.48687000  
C -3.35555000 -1.04534300 -1.23975500  
C -2.09090100 -2.76744400 0.00000000  
C -3.06977800 -1.71064000 0.00000000  
C -1.45031000 -3.10485900 1.23911600  
C -2.07286800 -2.74235100 2.48706700  
C -0.01702600 -3.35876600 3.72422100  
C -1.43688300 -3.08849100 3.73090400  
C 0.71938900 -3.30410200 4.95061700  
C -0.04213700 -3.41708800 6.17106200  
C -3.43250000 -1.01326800 -6.17961200  
C -2.07396300 -2.76005800 -4.96888900  
C -3.06882100 -1.70980000 -4.96762400  
C -1.43688300 -3.08849100 -3.73090400  
C -2.07286800 -2.74235100 -2.48706700  
C -0.04312300 -3.36458600 -1.23599400

C -1.45031000 -3.10485900 -1.23911600  
C 0.67140500 -3.29434800 0.00000000  
C -0.04312300 -3.36458600 1.23599400  
C 1.98244900 -2.68097400 2.46705800  
C 0.68291600 -3.26112300 2.47659200  
C 2.58136800 -2.26312100 3.69983400  
C 2.05938500 -2.75778900 4.93387800  
C 3.44615700 -1.15637400 6.14676000  
C 2.71602500 -2.32085000 6.14697100  
C -0.04213700 -3.41708800 -6.17106200  
C -1.39467900 -3.15476000 -6.17988700  
C 0.71938900 -3.30410200 -4.95061700  
C -0.01702600 -3.35876600 -3.72422100  
C 1.98244900 -2.68097400 -2.46705800  
C 0.68291600 -3.26112300 -2.47659200  
C 2.52510400 -2.21139500 -1.22605900  
C 1.98495100 -2.69789000 0.00000000  
C 3.40627100 -1.08127800 1.17539200  
C 2.52510400 -2.21139500 1.22605900  
C 3.58212200 -0.35047500 2.44617700  
C 3.38375000 -1.04824600 3.68439300  
C 3.41802700 1.06360600 4.97443800  
C 3.57028800 -0.36797300 4.94189500  
C 3.10768700 1.77891600 6.19225900  
C 2.71602500 -2.32085000 -6.14697100  
C 2.05938500 -2.75778900 -4.93387800  
C 3.38375000 -1.04824600 -3.68439300

C 2.58136800 -2.26312100 -3.69983400  
C 3.58212200 -0.35047500 -2.44617700  
C 3.40627100 -1.08127800 -1.17539200  
N 3.82718800 -0.54356800 0.00000000  
N 3.06939200 1.71424500 1.30899600  
C 3.37026900 1.07820500 2.48043400  
C 3.07626500 1.70215000 3.74486000  
C 3.44615700 -1.15637400 -6.14676000  
C 3.41802700 1.06360600 -4.97443800  
C 3.57028800 -0.36797300 -4.94189500  
C 3.07626500 1.70215000 -3.74486000  
C 3.37026900 1.07820500 -2.48043400  
N 3.06939200 1.71424500 -1.30899600  
C 3.10768700 1.77891600 -6.19225900  
H 3.53829200 1.44689900 7.14014900  
H 1.84271300 3.21694300 7.14098000  
H -0.29768200 3.68105100 7.12964600  
H -2.56850000 2.75340800 7.12141400  
H -3.71894000 0.88497300 7.12180500  
H -3.46659700 -1.55740000 7.12629200  
H -1.92763900 -3.11749100 7.13268200  
H 0.47602800 -3.58744700 7.11735400  
H 2.53165000 -2.84739400 7.08603500  
H 3.82806100 -0.75677000 7.08941300  
H -1.92763900 -3.11749100 -7.13268200  
H -3.46659700 -1.55740000 -7.12629200  
H -3.71894000 0.88497300 -7.12180500

H -2.56850000 2.75340800 -7.12141400  
H -0.29768200 3.68105100 -7.12964600  
H 1.84271300 3.21694300 -7.14098000  
H 3.53829200 1.44689900 -7.14014900  
H 3.82806100 -0.75677000 -7.08941300  
H 2.53165000 -2.84739400 -7.08603500  
H 0.47602800 -3.58744700 -7.11735400

**the coordiantes of N3 group on (5,5) SWCNT**

C -1.81942800 -0.22958800 -3.41996000  
C -3.05998800 -0.95314800 -3.30355100  
C -4.30441800 -0.27178500 -3.44895700  
C -5.47690800 -2.31258500 -2.78031300  
C -5.48909100 -1.08520600 -3.41712600  
C 3.14670900 -0.23368900 -3.46837300  
C 1.89831900 -0.93968700 -3.32821800  
C 0.65671400 -0.23133700 -3.46171700  
C -0.56421600 -2.21848200 -2.65135200  
C -0.57546200 -0.94074100 -3.32400000  
C -1.79758800 -2.72304500 -2.12038700  
C -3.04725600 -2.24075600 -2.64283000  
C -4.27235900 -3.42559500 -0.85026200  
C -4.27260400 -2.79533300 -2.16535100  
C -5.47987700 -3.55926600 -0.08487400  
C 5.58434700 -0.18828900 -3.57121800  
C 4.38714200 -2.23529600 -2.70418400

C 4.37986100 -0.94964400 -3.39686700  
C 3.15829500 -2.70183100 -2.14756000  
C 1.90666800 -2.19969400 -2.65436100  
C 0.67822600 -3.35717200 -0.84685600  
C 0.67131000 -2.71844700 -2.14150300  
C -0.55085600 -3.47070400 -0.13125700  
C -1.79296200 -3.35915200 -0.84191900  
C -3.03955200 -3.22956900 1.29274800  
C -3.03959700 -3.47742000 -0.13093100  
C -4.27220300 -2.93838200 1.95276700  
C -5.47983700 -3.32210700 1.27770800  
C 5.60339900 -3.38692100 -0.91892300  
C 5.59700900 -2.79053400 -2.16731400  
C 4.39994500 -3.46454100 -0.14100800  
C 3.16534600 -3.32963700 -0.84556400  
C 1.92004900 -3.18556900 1.27618000  
C 1.91998800 -3.43069700 -0.13057600  
C 0.67831000 -2.87525800 1.92581400  
C -0.55080600 -3.22291400 1.29034300  
C -1.79737000 -1.84912400 2.91154900  
C -1.79284500 -2.87886700 1.92205000  
C -3.04693300 -1.21929500 3.24171200  
C -4.27230600 -1.90203200 2.97881500  
C -5.48875700 0.12931300 3.58337600  
C -5.47651100 -1.24063500 3.39603600  
C 5.60357000 -2.87876000 2.00366600  
C 4.40005900 -3.21391300 1.29753900

C 3.15842500 -1.81984300 2.92978100  
C 3.16544100 -2.84962500 1.91528700  
C 1.90679300 -1.17669700 3.23834500  
C 0.67147700 -1.83753600 2.92951800  
C -0.57533800 0.23393000 3.44550700  
C -0.56403800 -1.19551500 3.24200000  
C -1.81934000 0.93622100 3.29823000  
C -3.05975900 0.21539200 3.43062200  
C -4.34104900 2.16874400 2.58923200  
C -4.30420700 0.90622600 3.33971100  
C -5.55087300 2.45530900 1.87784800  
C 5.59715400 -1.89672500 2.97835100  
C 4.38000300 0.25032800 3.51714300  
C 4.38725400 -1.19327300 3.29712900  
C 3.14678600 0.94873500 3.34506700  
C 1.89843300 0.23644700 3.44906800  
C 0.65417300 2.22806800 2.66678000  
C 0.65675900 0.94866000 3.33838300  
C -0.57807400 2.73217200 2.14777500  
C -1.83200000 2.21670800 2.65347500  
C -3.03189200 3.40639400 0.86252800  
C -3.07769700 2.71515600 2.13590500  
C -4.21339200 3.49785200 0.11782900  
C -5.49340200 3.02934700 0.59697600  
N -6.35012100 2.63900800 -0.45729800  
C 5.58506500 2.24560700 2.77346400  
C 5.58431600 1.02651800 3.42676900

C 4.38153600 2.75294800 2.17862600  
C 3.14719500 2.22316400 2.66450300  
C 1.90967600 3.33095000 0.84868600  
C 1.89945400 2.71289200 2.13590900  
C 0.67415800 3.45370200 0.13508200  
C -0.55778500 3.36393100 0.84904300  
C -1.79071900 3.23049400 -1.29020600  
C -1.79076600 3.47755400 0.12832500  
C -3.03173000 2.91653000 -1.95773300  
C -4.21316900 3.25288500 -1.28744300  
C -5.55070600 1.67917400 -2.59431500  
C -5.49314500 2.65057200 -1.58096300  
C 5.59638500 3.50921800 0.09437100  
C 4.38900100 3.37873600 0.85871800  
C 3.15861400 3.18524100 -1.28467600  
C 3.15859500 3.43303100 0.13855700  
C 1.90970100 2.84995300 -1.91879800  
C 0.67417600 3.20566000 -1.28827000  
C -0.57794700 1.84837000 -2.94024900  
C -0.55773400 2.88096100 -1.93037400  
C -1.83187400 1.19307800 -3.24360700  
C -3.07744900 1.83651500 -2.92388800  
C -4.34084700 1.16974100 -3.16744900  
C 5.59639600 3.27183000 -1.26912300  
C 4.38154300 1.85733600 -2.97629400  
C 4.38897800 2.89132700 -1.94440200  
C 3.14716500 1.19523000 -3.25587400

C 1.89952300 1.83421800 -2.92259700  
C 0.65424700 1.19932400 -3.25978100  
C 5.58510600 1.17936700 -3.36540500  
H 6.53506100 0.59126200 3.74303900  
H 6.54713700 -1.55869800 3.39857300  
H 6.55847300 -3.29588000 1.67571600  
H 6.55819800 -3.66930300 -0.46940100  
H 6.54706200 -2.61376200 -2.67659500  
H 6.53505400 -0.70496500 -3.72196300  
H 6.53650600 1.71617100 -3.35798700  
H 6.54940400 3.23567700 -1.80181700  
H 6.54946700 3.65533000 0.60775500  
H 6.53633000 2.74911800 2.58641800  
H -6.46784300 1.09308600 -2.66662000  
H -6.43624100 -0.67760700 -3.77864600  
H -6.41670000 -2.85126400 -2.63726900  
H -6.43312200 -3.69933800 -0.59967300  
H -6.43294700 -3.27981800 1.80980500  
H -6.41625600 -1.79603900 3.44309500  
H -6.43573300 0.63473500 3.78772100  
H -6.46778900 1.92704400 2.14240600

**the coordiantes of N0 group on (9,0) SWCNT**

C -1.75848600 -5.72698400 3.09656600  
C 0.65221600 -5.72191000 3.54012300  
C 2.76430600 -5.71636600 2.27173400



N 3.54736900 -5.73165400 0.00000000  
C 2.76430600 -5.71636600 -2.27173400  
C 0.65221600 -5.72191000 -3.54012300  
C -1.75848600 -5.72698400 -3.09656600  
C -3.31263000 -5.72971600 -1.21635000  
C -3.31263000 -5.72971600 1.21635000  
C -0.59686100 -5.03522200 3.52590700  
C 1.81460300 -5.03601500 3.08244300  
C 3.32720000 -5.02732700 1.16086800  
C 3.32720000 -5.02732700 -1.16086800  
C 1.81460300 -5.03601500 -3.08244300  
C -0.59686100 -5.03522200 -3.52590700  
C -2.72361500 -5.03463200 -2.30295100  
C -3.56778900 -5.03381100 0.00000000  
C -2.72361500 -5.03463200 2.30295100  
C -0.61716700 -3.58219000 3.53158700  
C 1.79675500 -3.58205800 3.09779200  
C 3.34441700 -3.57781800 1.21083400  
C 3.34441700 -3.57781800 -1.21083400  
C 1.79675500 -3.58205800 -3.09779200  
C -0.61716700 -3.58219000 -3.53158700  
C -2.75272700 -3.58613500 -2.31166800  
C -3.60640600 -3.58898900 0.00000000  
C -2.75272700 -3.58613500 2.31166800  
C -1.78598200 -2.87463700 3.10168700  
C 0.62675100 -2.86919700 3.52942900  
C 2.74350700 -2.86296600 2.30227000

C 3.57759700 -2.85245800 0.00000000  
C 2.74350700 -2.86296600 -2.30227000  
C 0.62675100 -2.86919700 -3.52942900  
C -1.78598200 -2.87463700 -3.10168700  
C -3.36552800 -2.87997100 -1.22601400  
C -3.36552800 -2.87997100 1.22601400  
C -1.78964500 -1.43884400 3.10486500  
C 0.62695700 -1.43282600 3.53089100  
C 2.74989900 -1.42668700 2.30469200  
C 3.59465100 -1.41947200 0.00000000  
C 2.74989900 -1.42668700 -2.30469200  
C 0.62695700 -1.43282600 -3.53089100  
C -1.78964500 -1.43884400 -3.10486500  
C -3.37088500 -1.44317800 -1.22711600  
C -3.37088500 -1.44317800 1.22711600  
C -0.62047300 -0.72023600 3.52711800  
C 1.79535500 -0.71288400 3.10475400  
C 3.37400800 -0.70807400 1.22734100  
C 3.37400800 -0.70807400 -1.22734100  
C 1.79535500 -0.71288400 -3.10475400  
C -0.62047300 -0.72023600 -3.52711800  
C -2.74499900 -0.72644300 -2.30238900  
C -3.58874000 -0.72879700 0.00000000  
C -2.74499900 -0.72644300 2.30238900  
C -0.62491900 0.71415500 3.52623700  
C 1.79114500 0.72123200 3.10446500  
C 3.36937000 0.72603600 1.22706800

C 3.36937000 0.72603600 -1.22706800  
C 1.79114500 0.72123200 -3.10446500  
C -0.62491900 0.71415500 -3.52623700  
C -2.74998700 0.70785300 -2.30230300  
C -3.59431900 0.70493000 0.00000000  
C -2.74998700 0.70785300 2.30230300  
C -1.79802900 1.42627000 3.10381900  
C 0.61796300 1.43394700 3.52790900  
C 2.74056700 1.44014900 2.30334900  
C 3.57848700 1.44175200 0.00000000  
C 2.74056700 1.44014900 -2.30334900  
C 0.61796300 1.43394700 -3.52790900  
C -1.79802900 1.42627000 -3.10381900  
C -3.38035000 1.42053800 -1.22715900  
C -3.38035000 1.42053800 1.22715900  
C -1.80367600 2.86180800 3.09989700  
C 0.60935700 2.86939200 3.52270500  
C 2.73122300 2.87554600 2.30129100  
C 3.57111400 2.87769300 0.00000000  
C 2.73122300 2.87554600 -2.30129100  
C 0.60935700 2.86939200 -3.52270500  
C -1.80367600 2.86180800 -3.09989700  
C -3.38533100 2.85744900 -1.22602800  
C -3.38533100 2.85744900 1.22602800  
C -0.63821300 3.57657300 3.52314900  
C 1.77518600 3.58833800 3.09270100  
C 3.35008300 3.59586600 1.22159900

C 3.35008300 3.59586600 -1.22159900  
C 1.77518600 3.58833800 -3.09270100  
C -0.63821300 3.57657300 -3.52314900  
C -2.77755200 3.56741800 -2.31092100  
C -3.63598900 3.56442700 0.00000000  
C -2.77755200 3.56741800 2.31092100  
C -0.62561900 5.03003300 3.52056100  
C 1.78967800 5.04133800 3.09602400  
C 3.36758000 5.04605000 1.22334000  
C 3.36758000 5.04605000 -1.22334000  
C 1.78967800 5.04133800 -3.09602400  
C -0.62561900 5.03003300 -3.52056100  
C -2.75537400 5.01550000 -2.30190000  
C -3.60440600 5.00800100 0.00000000  
C -2.75537400 5.01550000 2.30190000  
C -1.79440100 5.71446900 3.09598200  
C 0.61970700 5.72106800 3.54820200  
C 2.76879300 5.72461500 2.32869300  
C 3.62278300 5.72530700 0.00000000  
C 2.76879300 5.72461500 -2.32869300  
C 0.61970700 5.72106800 -3.54820200  
C -1.79440100 5.71446900 -3.09598200  
C -3.34994000 5.70645500 -1.21578500  
C -3.34994000 5.70645500 1.21578500  
H -1.78825700 6.80884700 3.07100400  
H 0.61040600 6.81529900 3.52907300  
H 2.74634400 6.81857200 2.31293000

H 3.59060600 6.81905900 0.00000000  
H 2.74634400 6.81857200 -2.31293000  
H 0.61040600 6.81529900 -3.52907300  
H -1.78825700 6.80884700 -3.07100400  
H -3.31857400 6.80095700 -1.20044400  
H -3.31857400 6.80095700 1.20044400  
H -1.74380400 -6.82124900 3.06971200  
H 0.64698900 -6.81592900 3.51285400  
H 2.72378300 -6.80575700 2.19835200  
H 2.72378300 -6.80575700 -2.19835200  
H 0.64698900 -6.81592900 -3.51285400  
H -1.74380400 -6.82124900 -3.06971200  
H -3.27435900 -6.82394600 -1.20173300  
H -3.27435900 -6.82394600 1.20173300

**the coordiantes of N1 group on (9,0) SWCNT**

C -5.72126600 -0.62378900 -3.48608700  
C -5.70362400 1.80528600 -3.05438400  
C -5.68704500 3.46418100 -1.22865400  
C -5.68704500 3.46419100 1.22862800  
C -5.70362400 1.80530900 3.05437000  
C -5.72126500 -0.62376300 3.48609200  
C -5.72106200 -2.77847200 2.30080300  
C -5.71904800 -3.64491700 0.00001400  
C -5.72106200 -2.77848900 -2.30078200  
C -5.02857800 0.61906400 -3.47076800

C -5.00713800 2.76854900 -2.27116900  
C -4.99089800 3.69885400 -0.00001400  
C -5.00713700 2.76856600 2.27114800  
C -5.02857700 0.61909000 3.47076400  
C -5.03272900 -1.80434800 3.08144800  
C -5.03123400 -3.40618400 1.22527800  
C -5.03123400 -3.40619300 -1.22525200  
C -5.03272900 -1.80437100 -3.08143400  
C -3.58200200 0.60923800 -3.48846800  
C -3.55664800 2.75064600 -2.27317700  
C -3.55885300 3.70232600 -0.00001400  
C -3.55664800 2.75066300 2.27315700  
C -3.58200200 0.60926500 3.48846300  
C -3.58617300 -1.81383700 3.09454700  
C -3.58183800 -3.40704700 1.22706100  
C -3.58183800 -3.40705600 -1.22703600  
C -3.58617300 -1.81386000 -3.09453300  
C -2.87199100 -0.63648000 -3.49866700  
C -2.86202200 1.77302400 -3.05472900  
C -2.83543000 3.41000600 -1.21749300  
C -2.83542900 3.41001500 1.21746700  
C -2.86202200 1.77304700 3.05471500  
C -2.87199000 -0.63645400 3.49867100  
C -2.87027700 -2.77290100 2.29848600  
C -2.86754600 -3.62391900 0.00001400  
C -2.87027800 -2.77291800 -2.29846500  
C -1.43487800 -0.64316600 -3.51267400

C -1.43202800 1.76628700 -3.06704700  
C -1.42049100 3.35955200 -1.21336100  
C -1.42049100 3.35956100 1.21333500  
C -1.43202800 1.76631000 3.06703400  
C -1.43487800 -0.64313900 3.51267900  
C -1.43457000 -2.77717400 2.30262500  
C -1.43404800 -3.62545400 0.00001400  
C -1.43457000 -2.77719100 -2.30260400  
C -0.71647000 0.59879300 -3.50264900  
C -0.71242300 2.70373500 -2.25723200  
N -0.69836300 3.63334400 -0.00001400  
C -0.71242300 2.70375200 2.25721100  
C -0.71647000 0.59882000 3.50264400  
C -0.71749900 -1.81871600 3.10127100  
C -0.71813800 -3.40134700 1.22656700  
C -0.71813800 -3.40135600 -1.22654200  
C -0.71750000 -1.81873900 -3.10125700  
C 0.71513500 0.60047700 -3.50066800  
C 0.71694200 2.71900000 -2.27381100  
C 0.70167300 3.62033700 -0.00001400  
C 0.71694200 2.71901700 2.27379100  
C 0.71513500 0.60050300 3.50066300  
C 0.71474500 -1.81724900 3.09990000  
C 0.71667900 -3.40091700 1.22638400  
C 0.71667900 -3.40092600 -1.22635900  
C 0.71474500 -1.81727200 -3.09988700  
C 1.43177900 -0.63923100 -3.50730900

C 1.42893600 1.77303900 -3.06533700  
C 1.41894100 3.40560200 -1.22196900  
C 1.41894100 3.40561100 1.22194300  
C 1.42893600 1.77306200 3.06532300  
C 1.43177900 -0.63920500 3.50731300  
C 1.43261900 -2.77442300 2.30180900  
C 1.43268000 -3.62313300 0.00001400  
C 1.43261900 -2.77444000 -2.30178800  
C 2.86914900 -0.63211300 -3.49662900  
C 2.86452700 1.78170200 -3.06313200  
C 2.85418700 3.40952000 -1.21927900  
C 2.85418700 3.40953000 1.21925300  
C 2.86452700 1.78172500 3.06311900  
C 2.86914900 -0.63208700 3.49663400  
C 2.86806400 -2.76786200 2.29792400  
C 2.86673200 -3.61885500 0.00001300  
C 2.86806400 -2.76787900 -2.29790300  
C 3.57932900 0.61646100 -3.49414000  
C 3.56802600 2.76005000 -2.28635600  
C 3.57036900 3.65110300 -0.00001400  
C 3.56802600 2.76006700 2.28633500  
C 3.57932900 0.61648800 3.49413500  
C 3.58228000 -1.80595200 3.09215500  
C 3.58080500 -3.40097800 1.22682300  
C 3.58080500 -3.40098800 -1.22679800  
C 3.58228000 -1.80597500 -3.09214200  
C 5.02748800 0.62115500 -3.48910600



C 5.01819000 2.76342300 -2.28647400  
C 5.01766600 3.64276000 -0.00001400  
C 5.01819000 2.76344000 2.28645400  
C 5.02748800 0.62118100 3.48910100  
C 5.03082600 -1.79969000 3.08476000  
C 5.03026700 -3.39738100 1.22508200  
C 5.03026700 -3.39739000 -1.22505700  
C 5.03082600 -1.79971300 -3.08474700  
C 5.71806100 -0.62472300 -3.50430500  
C 5.70908400 1.80238600 -3.07864700  
C 5.70601200 3.42405300 -1.22747600  
C 5.70601200 3.42406300 1.22745100  
C 5.70908400 1.80241000 3.07863400  
C 5.71806100 -0.62469600 3.50431000  
C 5.71913200 -2.77137500 2.30357600  
C 5.71829900 -3.62981800 0.00001400  
C 5.71913200 -2.77139200 -2.30355600  
H 6.81218900 -0.61845000 -3.47478800  
H 6.80322600 1.79269600 -3.05163500  
H 6.80019300 3.39991600 -1.21806900  
H 6.80019300 3.39992600 1.21804500  
H 6.80322600 1.79272000 3.05162300  
H 6.81218900 -0.61842300 3.47479300  
H 6.81332900 -2.74971000 2.28431500  
H 6.81247900 -3.60180300 0.00001300  
H 6.81332900 -2.74972800 -2.28429500  
H -6.81514200 -0.61642800 -3.44861200

H -6.79771900 1.80168300 -3.02643400  
H -6.78120800 3.45166500 -1.21663600  
H -6.78120800 3.45167400 1.21661000  
H -6.79771900 1.80170500 3.02642100  
H -6.81514200 -0.61640200 3.44861700  
H -6.81518100 -2.75533700 2.27934200  
H -6.81327800 -3.61987000 0.00001400  
H -6.81518100 -2.75535400 -2.27932100

**the coordiantes of N2 group on (9,0) SWCNT**

C 5.71500900 1.78701900 3.12019200  
C 5.75200900 3.36505800 1.23554000  
C 5.75200900 3.36570800 -1.23374100  
C 5.71500200 1.78864500 -3.11914300  
C 5.68699800 -0.63072000 -3.53675000  
C 5.69166700 -2.76510800 -2.30993100  
C 5.69630600 -3.61458800 -0.00093500  
C 5.69162000 -2.76626200 2.30845700  
C 5.68696300 -0.63259200 3.53645500  
C 5.04758000 2.75066400 2.31433000  
C 5.07553300 3.57362400 0.00089000  
C 5.04748500 2.75208500 -2.31306500  
C 5.00589400 0.62059400 -3.52019900  
C 5.00098200 -1.79658000 -3.09286100  
C 5.00729600 -3.38845700 -1.22666800  
C 5.00721300 -3.38921700 1.22504300

C 5.00086400 -1.79835400 3.09211000  
C 5.00590900 0.61863500 3.52050900  
C 3.59936700 2.77330300 2.31028500  
C 3.62331400 3.59185600 0.00088000  
C 3.59939800 2.77479800 -2.30906300  
C 3.55566200 0.63178400 -3.49358100  
C 3.55252600 -1.79048200 -3.08185300  
C 3.55844500 -3.39725700 -1.22709600  
C 3.55844900 -3.39807900 1.22546200  
C 3.55251200 -1.79231100 3.08114700  
C 3.55563400 0.62979800 3.49386100  
C 2.85696300 1.80553200 3.06478600  
C 2.90686800 3.39930800 1.22501500  
C 2.90687900 3.40006700 -1.22329500  
C 2.85699100 1.80718600 -3.06386600  
C 2.84177500 -0.61453300 -3.48119300  
C 2.84247200 -2.75924100 -2.29211000  
C 2.84527200 -3.62193700 -0.00094200  
C 2.84245400 -2.76045000 2.29069200  
C 2.84174700 -0.61636900 3.48092200  
C 1.40974600 1.82175600 3.03644100  
C 1.46725300 3.37988900 1.16965400  
C 1.46724500 3.38058100 -1.16790100  
C 1.40971900 1.82340800 -3.03549300  
C 1.40646100 -0.60817800 -3.46489700  
C 1.40857400 -2.76535700 -2.29151800  
C 1.41136600 -3.63403200 -0.00094700

C 1.40851800 -2.76658800 2.29008700  
C 1.40643100 -0.61004400 3.46461900  
C 0.70862000 2.81269300 2.27856700  
N 0.80892000 3.51629600 0.00087300  
C 0.70860800 2.81397500 -2.27722500  
C 0.69530600 0.63454100 -3.45113600  
C 0.69078900 -1.79216900 -3.06749500  
C 0.69369500 -3.41225900 -1.22670100  
C 0.69366900 -3.41293600 1.22495900  
C 0.69075000 -1.79383900 3.06659000  
C 0.69529400 0.63266800 3.45142200  
C -0.74510800 2.81276900 2.25858100  
C -0.74509300 2.81402900 -2.25718900  
C -0.73215600 0.62064500 -3.42494900  
C -0.74030700 -1.79986500 -3.06663600  
C -0.74075100 -3.41749900 -1.22683800  
C -0.74076200 -3.41817700 1.22506300  
C -0.74033600 -1.80152100 3.06573100  
C -0.73218200 0.61881400 3.42524900  
C -1.43522600 1.78493100 2.99484000  
N -1.41884500 3.62418400 1.40001800  
N -1.41881700 3.62495400 -1.39811600  
C -1.43521300 1.78653600 -2.99392800  
C -1.45326600 -0.61778200 -3.45108600  
C -1.45787900 -2.77789700 -2.29301900  
C -1.45752400 -3.64715900 -0.00096200  
C -1.45790400 -2.77910900 2.29156000

C -1.45329500 -0.61960800 3.45077400  
C -2.86041100 1.80122200 3.00403300  
C -2.76941300 3.51707700 1.26887600  
C -2.76938100 3.51776800 -1.26701600  
C -2.86039300 1.80280700 -3.00307100  
C -2.88958400 -0.60646800 -3.44148500  
C -2.89348900 -2.76946600 -2.28715100  
C -2.89113600 -3.64608700 -0.00096700  
C -2.89351700 -2.77066400 2.28567700  
C -2.88961100 -0.60828600 3.44117200  
C -3.54740500 2.78918100 2.23544800  
C -3.45421700 3.81277300 0.00101100  
C -3.54738000 2.79035300 -2.23396000  
C -3.59279500 0.64019600 -3.42793600  
C -3.60795500 -1.78723300 -3.05579400  
C -3.60583800 -3.42130700 -1.22703600  
C -3.60585500 -3.42194800 1.22521600  
C -3.60798600 -1.78884500 3.05483700  
C -3.59281500 0.63838700 3.42827600  
C -4.99063600 2.82573400 2.23915100  
C -4.89592700 3.80693200 0.00100400  
C -4.99061300 2.82691500 -2.23765700  
C -5.03854900 0.65947200 -3.40533400  
C -5.05461500 -1.77082400 -3.04240200  
C -5.05443400 -3.41503600 -1.22521900  
C -5.05444800 -3.41567200 1.22338600  
C -5.05464300 -1.77242300 3.04144200

C -5.03857400 0.65767800 3.40568600  
C -5.70419200 1.85360900 2.99576500  
C -5.62837400 3.56846300 1.21180000  
C -5.62836200 3.56912700 -1.20993700  
C -5.70416900 1.85519000 -2.99478000  
C -5.73792200 -0.57916400 -3.42403900  
C -5.74446500 -2.76321200 -2.28616200  
C -5.74277100 -3.66041900 -0.00098600  
C -5.74449200 -2.76439700 2.28466100  
C -5.73794900 -0.58096800 3.42372600  
H -6.79839600 1.86404900 2.97151700  
H -6.72160100 3.59673600 1.17462400  
H -6.72158900 3.59740700 -1.17276500  
H -6.79837300 1.86562900 -2.97054400  
H -6.83157300 -0.56696500 -3.38301100  
H -6.83844000 -2.73752000 -2.26220800  
H -6.83699400 -3.63351800 -0.00098600  
H -6.83846700 -2.73869400 2.26071400  
H -6.83160000 -0.56874400 3.38270400  
H 6.80914500 1.75715400 3.10828500  
H 6.84591000 3.32417600 1.23460200  
H 6.84589900 3.32464400 -1.23301300  
H 6.80913300 1.75880900 -3.10702300  
H 6.78151400 -0.63042800 -3.52791800  
H 6.78600100 -2.74667700 -2.29827200  
H 6.79045300 -3.58478000 -0.00078000  
H 6.78594500 -2.74762400 2.29670400

H 6.78147800 -0.63255200 3.52752500

**the coordiantes of N0 group on (11,0) SWCNT**

C -5.71813600 -3.78864300 2.17393100

C -5.72672200 -4.36447400 -0.21776700

C -5.73786800 -3.53782500 -2.53660100

C -5.74573900 -1.58517000 -4.03834100

C -5.74623000 0.86959500 -4.24871800

C -5.73899000 3.04930700 -3.10138100

C -5.72792600 4.26062700 -0.95832500

C -5.71913000 4.10431400 1.49675100

C -5.70924700 2.61351100 3.45565400

N -5.71866100 0.36795400 4.28076500

C -5.70866300 -1.98503700 3.84941700

C -5.03371200 -4.25009000 1.01735600

C -5.04437300 -4.11425000 -1.43859900

C -5.05479500 -2.66542700 -3.42617900

C -5.05930000 -0.37245800 -4.31578800

C -5.05563100 2.03839300 -3.82966800

C -5.04556900 3.80489500 -2.11826400

C -5.03494600 4.36021300 0.27807400

C -5.02786500 3.50865600 2.58624600

C -5.01076300 1.51817300 4.02617900

C -5.01044600 -0.80870600 4.22533400

C -5.02706900 -3.01550900 3.14553400

C -3.58162500 -4.25685700 1.01100000

C -3.59246800 -4.11618400 -1.44584500  
C -3.60259600 -2.66681900 -3.43449500  
C -3.60695300 -0.37297000 -4.32515500  
C -3.60334500 2.03899900 -3.83844400  
C -3.59379700 3.80618300 -2.12600100  
C -3.58299000 4.36626800 0.27043800  
C -3.57447600 3.53115400 2.58431400  
C -3.56081400 1.57127900 4.05780600  
C -3.56049100 -0.85555200 4.26567800  
C -3.57365100 -3.03785600 3.14764400  
C -2.86582800 -3.79979400 2.16373300  
C -2.87575900 -4.35771000 -0.23022100  
C -2.88661500 -3.52976700 -2.54457600  
C -2.89406800 -1.58194200 -4.04379400  
C -2.89448400 0.86695600 -4.25388000  
C -2.88767900 3.04160000 -3.10831900  
C -2.87715000 4.25305400 -0.96973700  
C -2.86694200 4.11425700 1.48423300  
C -2.85480400 2.66499500 3.46646100  
C -2.83986900 0.37403800 4.34677700  
C -2.85429200 -2.03339700 3.86959700  
C -1.42622600 -3.80185100 2.15878800  
C -1.43715600 -4.35931000 -0.23699600  
C -1.44819200 -3.53146400 -2.55295500  
C -1.45550100 -1.58318100 -4.05365300  
C -1.45591300 0.86688500 -4.26385400  
C -1.44923300 3.04218900 -3.11687800



C -1.43844800 4.25392900 -0.97677100  
C -1.42727600 4.11586900 1.47891000  
C -1.41556200 2.66912700 3.46745700  
C -1.40471800 0.37527700 4.36017700  
C -1.41494600 -2.03704200 3.87149100  
C -0.71684100 -4.25234700 0.99736500  
C -0.72857900 -4.11119900 -1.45770400  
C -0.73804200 -2.66498600 -3.44635200  
C -0.74194600 -0.37340200 -4.33763700  
C -0.73875000 2.03632000 -3.84977100  
C -0.72961600 3.80026500 -2.13684200  
C -0.71789700 4.36050400 0.25753200  
C -0.70542200 3.53516700 2.57336200  
C -0.69571800 1.58661700 4.07335800  
C -0.69545600 -0.86716300 4.28420400  
C -0.70473400 -3.04292000 3.13805000  
C 0.72023900 -4.25235300 0.98974100  
C 0.70793200 -4.11096600 -1.46499000  
C 0.69852100 -2.66510600 -3.45380900  
C 0.69474200 -0.37375500 -4.34545900  
C 0.69788100 2.03588100 -3.85732900  
C 0.70679800 3.79962100 -2.14418000  
C 0.71903200 4.36001800 0.24994300  
C 0.73166500 3.53479800 2.56549600  
C 0.74041500 1.58562100 4.06407500  
C 0.74064400 -0.86715300 4.27469500  
C 0.73241800 -3.04321600 3.13012400

C 1.44159500 -3.80193900 2.14316500  
C 1.42861000 -4.35852100 -0.25144700  
C 1.41724200 -3.53127400 -2.56703700  
C 1.41035100 -1.58392900 -4.06870300  
C 1.41001900 0.86616000 -4.27920100  
C 1.41637700 3.04123400 -3.13144400  
C 1.42747700 4.25270800 -0.99126500  
C 1.44070800 4.11516200 1.46363200  
C 1.45173500 2.66810400 3.45119000  
C 1.45535700 0.37385400 4.33906200  
C 1.45211300 -2.03765900 3.85486400  
C 2.88023600 -3.79929000 2.13310200  
C 2.86725900 -4.35677500 -0.25975800  
C 2.85577200 -3.52978700 -2.57363500  
C 2.84895800 -1.58301300 -4.07365100  
C 2.84864600 0.86580000 -4.28403900  
C 2.85498600 3.03998300 -3.13771000  
C 2.86632800 4.25086100 -0.99907500  
C 2.87953600 4.11217100 1.45427700  
C 2.89014400 2.66571300 3.44063400  
C 2.89404800 0.37403500 4.32870000  
C 2.89049300 -2.03553400 3.84364700  
C 3.58641700 -4.25393700 0.97357400  
C 3.57302300 -4.11454900 -1.48143300  
C 3.56333900 -2.66775500 -3.47096000  
C 3.55942100 -0.37461600 -4.36330900  
C 3.56207700 2.03789900 -3.87676600

C 3.57111100 3.80478700 -2.16287400  
C 3.58439000 4.36429100 0.23398300  
C 3.59742400 3.53535200 2.55059500  
C 3.60462800 1.58482000 4.05009500  
C 3.60515300 -0.86659000 4.25764800  
C 3.59901200 -3.04224300 3.11238100  
C 5.03888000 -4.25723200 0.96685500  
C 5.02521400 -4.11665900 -1.48870900  
C 5.01559000 -2.66872200 -3.47738700  
C 5.01172500 -0.37577100 -4.36811400  
C 5.01423800 2.03526400 -3.88108700  
C 5.02291100 3.80097800 -2.16845200  
C 5.03652400 4.36048600 0.22663300  
C 5.04975500 3.53245300 2.54214700  
C 5.05658300 1.58345200 4.04240300  
C 5.05746500 -0.86842400 4.25192600  
C 5.05150600 -3.04512700 3.10667200  
C 5.73187700 -3.81641200 2.12646700  
C 5.71830400 -4.37524800 -0.27546400  
C 5.70662500 -3.54355600 -2.59612000  
C 5.70020100 -1.58926100 -4.09808700  
C 5.70001600 0.86578500 -4.30698300  
C 5.70602100 3.04432500 -3.15822000  
C 5.71754700 4.25808800 -1.01611300  
C 5.73143600 4.11984600 1.44266800  
C 5.74160300 2.67040300 3.43540500  
C 5.74418700 0.37319800 4.32826900

C 5.74170900 -2.04458500 3.84280500  
H 6.82601700 -3.80050900 2.11108200  
H 6.81252000 -4.35695500 -0.28054500  
H 6.80091000 -3.52793800 -2.58993800  
H 6.79452000 -1.58198900 -4.08433100  
H 6.79435300 0.86143600 -4.29135300  
H 6.80034700 3.02901600 -3.14790300  
H 6.81180000 4.23649200 -1.01711300  
H 6.82558100 4.09939400 1.42904100  
H 6.83571600 2.65732900 3.41333700  
H 6.83837200 0.37144500 4.30397400  
H 6.83582400 -2.03588000 3.82088100  
H -6.81198400 -3.75983500 2.16167400  
H -6.82090900 -4.34135100 -0.21154500  
H -6.83202000 -3.52107900 -2.51851200  
H -6.83983400 -1.57746900 -4.01324100  
H -6.84032100 0.86600100 -4.22244400  
H -6.83314300 3.03541100 -3.08038700  
H -6.82211600 4.23843600 -0.94803700  
H -6.81298000 4.07394700 1.48971100  
H -6.79887800 2.54279000 3.42176300  
H -6.79832000 -1.92141300 3.80413400

**the coordiantes of N1 group on (11,0) SWCNT**

C -5.72470700 -3.15079700 3.01621000  
C -5.71776500 -4.29045600 0.82418000

C -5.71005700 -4.08132000 -1.63435300  
C -5.71001900 -2.55922200 -3.57076000  
C -5.71763500 -0.22050000 -4.35766000  
C -5.72461700 2.18066300 -3.77573800  
C -5.72061400 3.89241400 -2.00136400  
C -5.71565800 4.36748700 0.41635200  
C -5.71398500 3.45270900 2.70661200  
C -5.71557900 1.44373600 4.13713000  
C -5.72053500 -1.01762000 4.25235500  
C -5.03674300 -3.86816800 1.99907200  
C -5.02618500 -4.34942500 -0.41558100  
C -5.02243500 -3.45518100 -2.70862200  
C -5.02612500 -1.43873100 -4.12009400  
C -5.03660700 1.02122400 -4.22833600  
C -5.03550200 3.15869600 -3.00878800  
C -5.02994000 4.29674500 -0.82603900  
C -5.02720500 4.06422900 1.62330400  
C -5.02714800 2.54452800 3.55668400  
C -5.02985200 0.22025500 4.36406300  
C -5.03550000 -2.17158200 3.78161100  
C -3.58618200 -3.87166200 2.00633000  
C -3.57405900 -4.34582100 -0.41187800  
C -3.57165000 -3.45371000 -2.70745400  
C -3.57401500 -1.43430500 -4.11738800  
C -3.58605800 1.02740000 -4.23327200  
C -3.58431200 3.16575600 -3.01526700  
C -3.57862000 4.29922400 -0.82990700

C -3.57594100 4.06241000 1.62044700  
C -3.57589400 2.54129800 3.55548600  
C -3.57852600 0.21703400 4.36718400  
C -3.58434700 -2.17627000 3.79003000  
C -2.87419500 -3.14767200 3.01903900  
C -2.87161800 -4.27339800 0.83241000  
C -2.86017300 -4.05541000 -1.62298400  
C -2.86017400 -2.54214900 -3.54831900  
C -2.87157500 -0.20853500 -4.34290600  
C -2.87410400 2.18408500 -3.77309200  
C -2.86989300 3.88618400 -2.00115600  
C -2.86468300 4.35187400 0.41179700  
C -2.86266700 3.43716500 2.69434500  
C -2.86463900 1.43558300 4.12292500  
C -2.86987600 -1.01900000 4.24610600  
C -1.43437800 -3.15652400 3.03042700  
C -1.43431300 -4.27469100 0.84127200  
C -1.42149200 -4.04187000 -1.61066500  
C -1.42150700 -2.52700400 -3.53811200  
C -1.43425200 -0.20027100 -4.34615700  
C -1.43432200 2.19294500 -3.78423700  
C -1.43133000 3.89152400 -2.00552800  
C -1.42763800 4.35361800 0.41108100  
C -1.42597100 3.43811600 2.69507500  
C -1.42760200 1.43525400 4.12467700  
C -1.43131700 -1.02201200 4.25225700  
C -0.72010200 -3.87419600 2.02379600

C -0.72295400 -4.30774200 -0.38880100  
C -0.70635100 -3.40791300 -2.67145100  
C -0.72295600 -1.40310600 -4.08619900  
C -0.72006400 1.04353100 -4.23937200  
C -0.71662100 3.17673400 -3.02228500  
C -0.71351100 4.29700500 -0.83225100  
C -0.71174000 4.05595800 1.61626800  
C -0.71174700 2.53572100 3.55014200  
C -0.71353100 0.21416300 4.36535600  
C -0.71663500 -2.18059100 3.80238900  
C 0.71370300 -3.87822700 2.02545300  
C 0.70987500 -4.28811200 -0.39289200  
N 0.70370700 -3.39783300 -2.66354700  
C 0.70990100 -1.40249900 -4.06637700  
C 0.71371200 1.04412000 -4.24359400  
C 0.71758200 3.17862600 -3.02575900  
C 0.72166500 4.29693100 -0.83446900  
C 0.72392300 4.05435600 1.61436700  
C 0.72391300 2.53348300 3.54904300  
C 0.72165000 0.21197100 4.36581400  
C 0.71754800 -2.18354400 3.80509800  
C 1.43252700 -3.16414300 3.03785100  
C 1.42969500 -4.27756900 0.84781300  
C 1.41658300 -3.98954800 -1.58293200  
C 1.41655300 -2.48800900 -3.49431300  
C 1.42966600 -0.19468200 -4.35044000  
C 1.43252200 2.19823800 -3.79329000

C 1.43545800 3.89268200 -2.00944500  
C 1.43827900 4.35093800 0.40838800  
C 1.43946500 3.43397300 2.69183700  
C 1.43821200 1.43199500 4.12275000  
C 1.43540700 -1.02555800 4.25432000  
C 2.87022100 -3.16063200 3.02745000  
C 2.85919800 -4.27680400 0.83985700  
C 2.84050800 -4.03515900 -1.61038800  
C 2.84050200 -2.52540500 -3.53206500  
C 2.85916900 -0.20222300 -4.34794000  
C 2.87016100 2.18901500 -3.78752600  
C 2.87412500 3.88624400 -2.00853100  
C 2.87493500 4.34703900 0.40747200  
C 2.87516300 3.43122300 2.68971300  
C 2.87486100 1.43020700 4.11930800  
C 2.87407000 -1.02618700 4.24797000  
C 3.57883600 -3.88129000 2.01475100  
C 3.55680800 -4.33820400 -0.40786700  
C 3.55933300 -3.45805600 -2.71093300  
C 3.55676800 -1.42875900 -4.11127600  
C 3.57872900 1.03314400 -4.24446300  
C 3.58591000 3.17055900 -3.02547700  
C 3.58722400 4.29555000 -0.83621000  
C 3.58763200 4.05481100 1.61397500  
C 3.58756400 2.53320200 3.54972300  
C 3.58708800 0.21000600 4.36515000  
C 3.58591600 -2.18508600 3.79721600



C 5.02824800 -3.87883400 1.99949600  
C 5.00839300 -4.35397500 -0.42089800  
C 4.99746100 -3.47236400 -2.72216900  
C 5.00835800 -1.44510700 -4.12354000  
C 5.02811900 1.01898700 -4.23869500  
C 5.03460100 3.15795600 -3.02022300  
C 5.03663300 4.29035900 -0.83544200  
C 5.03847400 4.05458900 1.61434000  
C 5.03839900 2.53351000 3.54952700  
C 5.03650200 0.20956600 4.36013800  
C 5.03457500 -2.18290300 3.78370400  
C 5.72085300 -3.16429700 3.01270800  
C 5.70382000 -4.30412200 0.81960500  
C 5.68821000 -4.09853900 -1.64251900  
C 5.68820000 -2.57132900 -3.58574500  
C 5.70371000 -0.22823900 -4.36991800  
C 5.72077100 2.17398000 -3.78797700  
C 5.72440400 3.88386800 -2.01101600  
C 5.72555200 4.35785500 0.40827800  
C 5.72608200 3.44309000 2.69911300  
C 5.72544100 1.43356700 4.12976900  
C 5.72429100 -1.02906000 4.24642200  
H 6.81488700 -3.14502200 2.99122600  
H 6.79797700 -4.29072800 0.80686200  
H 6.78237500 -4.08760400 -1.64351100  
H 6.78235600 -2.56950200 -3.57472500  
H 6.79786000 -0.23739700 -4.35404200

H 6.81481200 2.15773300 -3.76431600  
H 6.81854100 3.85875300 -1.99885200  
H 6.81979500 4.33616900 0.40540200  
H 6.82034300 3.42834700 2.68762400  
H 6.81968300 1.42556600 4.10946500  
H 6.81842100 -1.02318200 4.21909700  
H -6.81875200 -3.12993800 2.99730900  
H -6.81181700 -4.26655000 0.81394700  
H -6.80432100 -4.06361100 -1.62920800  
H -6.80427300 -2.54984200 -3.55465400  
H -6.81168300 -0.22473300 -4.33217800  
H -6.81866400 2.16723000 -3.75104100  
H -6.81488200 3.87295000 -1.98836900  
H -6.80995200 4.34697700 0.41579200  
H -6.80822600 3.43701900 2.69436900  
H -6.80987100 1.43827000 4.11740100  
H -6.81479700 -1.00959300 4.23031000

**the coordiantes of N2 group on (11,0) SWCNT**

C -5.69818700 0.59283500 -4.32604400  
C -5.74196100 2.83472500 -3.31394100  
C -5.78672800 4.16336200 -1.23800900  
C -5.78672800 4.16336800 1.23798700  
C -5.74196100 2.83474300 3.31392600  
C -5.69818700 0.59285800 4.32604000  
C -5.68558900 -1.84864700 3.97278300

C -5.68143400 -3.71826200 2.36329200  
C -5.68001000 -4.41707200 0.00001100  
C -5.68143400 -3.71827400 -2.36327400  
C -5.68558800 -1.84866800 -3.97277400  
C -5.02576800 1.79243400 -3.96360200  
C -5.07996300 3.66074500 -2.36853300  
C -5.11188400 4.33767800 -0.00001100  
C -5.07996300 3.66075800 2.36851400  
C -5.02576800 1.79245500 3.96359300  
C -5.00351400 -0.64590900 4.30352400  
C -4.99629000 -2.88925300 3.29097400  
C -4.99264500 -4.23239200 1.22983200  
C -4.99264500 -4.23239800 -1.22981100  
C -4.99629000 -2.88927100 -3.29096000  
C -5.00351400 -0.64593100 -4.30352200  
C -3.57360800 1.80576400 -3.93419600  
C -3.62969900 3.68811300 -2.36142000  
C -3.65791000 4.36251400 -0.00001100  
C -3.62969900 3.68812600 2.36140100  
C -3.57360800 1.80578500 3.93418700  
C -3.55232400 -0.63219200 4.28309100  
C -3.54450000 -2.88212100 3.28563200  
C -3.54221900 -4.23332700 1.22998400  
C -3.54221900 -4.23333400 -1.22996300  
C -3.54449900 -2.88213900 -3.28561800  
C -3.55232300 -0.63221400 -4.28308800  
C -2.85174600 0.61216700 -4.26339200

C -2.88266600 2.86171900 -3.25866700  
C -2.94021900 4.20984300 -1.22550300  
C -2.94021900 4.20985000 1.22548100  
C -2.88266700 2.86173700 3.25865300  
C -2.85174600 0.61219000 4.26338900  
C -2.83556400 -1.82616300 3.93794100  
C -2.83033200 -3.70418900 2.35339400  
C -2.82963500 -4.40972900 0.00001100  
C -2.83033100 -3.70420200 -2.35337500  
C -2.83556400 -1.82618400 -3.93793200  
C -1.41323900 0.62455900 -4.24028000  
C -1.43286000 2.88342300 -3.22734800  
C -1.49861000 4.19941900 -1.17042600  
C -1.49861100 4.19942600 1.17040400  
C -1.43286000 2.88344100 3.22733300  
C -1.41324000 0.62458100 4.24027700  
C -1.39879300 -1.81967700 3.93350100  
C -1.39359100 -3.70433600 2.35446500  
C -1.39246100 -4.41159700 0.00001100  
C -1.39359000 -3.70434800 -2.35444600  
C -1.39879200 -1.81969800 -3.93349200  
C -0.71220300 1.81643800 -3.88487800  
C -0.73716500 3.73967700 -2.32125400  
N -0.84208600 4.30956600 -0.00001100  
C -0.73716600 3.73969000 2.32123600  
C -0.71220300 1.81645800 3.88486900  
C -0.69001400 -0.61798900 4.25771600

C -0.67966300 -2.87543800 3.28168300  
C -0.67724500 -4.23055800 1.22966200  
C -0.67724500 -4.23056500 -1.22964000  
C -0.67966300 -2.87545500 -3.28166800  
C -0.69001300 -0.61801200 -4.25771300  
C 0.71846900 1.80781800 -3.85897400  
C 0.72108500 3.75903400 -2.31011700  
C 0.72108400 3.75904700 2.31009900  
C 0.71846800 1.80783900 3.85896500  
C 0.74296700 -0.61525800 4.25346100  
C 0.75549900 -2.87102000 3.27972400  
C 0.75834500 -4.22898600 1.22974800  
C 0.75834500 -4.22899300 -1.22972600  
C 0.75550000 -2.87103800 -3.27970900  
C 0.74296800 -0.61528100 -4.25345700  
C 1.44699000 0.63045500 -4.22024400  
C 1.41500700 2.85878600 -3.19428200  
N 1.39137600 4.47924900 -1.37756700  
N 1.39137600 4.47925600 1.37754300  
C 1.41500600 2.85880300 3.19426700  
C 1.44698900 0.63047800 4.22024100  
C 1.46651600 -1.81041400 3.92848000  
C 1.47326000 -3.69977000 2.35327500  
C 1.47408300 -4.41202400 0.00001100  
C 1.47326100 -3.69978300 -2.35325600  
C 1.46651600 -1.81043500 -3.92847100  
C 2.88397400 0.64666300 -4.20787000

C 2.84194400 2.88892900 -3.20747500  
C 2.74732300 4.38340800 -1.27115600  
C 2.74732300 4.38341500 1.27113400  
C 2.84194400 2.88894600 3.20746100  
C 2.88397400 0.64668500 4.20786700  
C 2.90462800 -1.79534900 3.91507300  
C 2.90987200 -3.69188500 2.35020800  
C 2.91005500 -4.40831100 0.00001100  
C 2.90987300 -3.69189800 -2.35018900  
C 2.90462900 -1.79537000 -3.91506400  
C 3.57852300 1.84527300 -3.86091700  
C 3.52543500 3.75801100 -2.30457000  
C 3.43283000 4.63210500 -0.00001200  
C 3.52543400 3.75802300 2.30455100  
C 3.57852200 1.84529400 3.86090700  
C 3.60982200 -0.58920000 4.23109100  
C 3.62161200 -2.85470000 3.27181800  
C 3.62269900 -4.22701700 1.23008300  
C 3.62269900 -4.22702400 -1.23006100  
C 3.62161200 -2.85471800 -3.27180300  
C 3.60982300 -0.58922300 -4.23108800  
C 5.02698200 1.86840300 -3.84307600  
C 4.96989700 3.79944300 -2.30662300  
C 4.87714000 4.63278000 -0.00001200  
C 4.96989700 3.79945600 2.30660400  
C 5.02698100 1.86842400 3.84306700  
C 5.05851300 -0.56983200 4.21249500

C 5.07101700 -2.84102400 3.26398900  
C 5.07286700 -4.22299300 1.22955300  
C 5.07286700 -4.22300000 -1.22953100  
C 5.07101700 -2.84104100 -3.26397400  
C 5.05851400 -0.56985400 -4.21249200  
C 5.73250300 0.68491100 -4.18709600  
C 5.68686200 2.95597800 -3.20012100  
C 5.60833400 4.43537200 -1.21447800  
C 5.60833300 4.43537800 1.21445600  
C 5.68686200 2.95599500 3.20010600  
C 5.73250200 0.68493300 4.18709300  
C 5.75484300 -1.76928000 3.89996200  
C 5.76083400 -3.68859300 2.35195000  
C 5.76103600 -4.41878800 0.00001200  
C 5.76083500 -3.68860500 -2.35193000  
C 5.75484300 -1.76930100 -3.89995300  
H 6.82641500 0.69309400 -4.15426000  
H 6.78101000 2.97234800 -3.17988000  
H 6.70149200 4.46574000 -1.17791800  
H 6.70149200 4.46574600 1.17789600  
H 6.78100900 2.97236500 3.17986600  
H 6.82641500 0.69311600 4.15425700  
H 6.84869500 -1.75134500 3.87034900  
H 6.85491700 -3.66586200 2.33741500  
H 6.85524700 -4.39785200 0.00001200  
H 6.85491800 -3.66587500 -2.33739600  
H 6.84869500 -1.75136600 -3.87033900

H -6.79261400 0.58344800 -4.32582700  
H -6.83595200 2.79962500 -3.31284600  
H -6.88047600 4.12241200 -1.24198800  
H -6.88047700 4.12241800 1.24196600  
H -6.83595200 2.79964300 3.31283100  
H -6.79261500 0.58347100 4.32582300  
H -6.77996400 -1.84863100 3.96606600  
H -6.77575100 -3.70570300 2.35329300  
H -6.77430400 -4.39739400 0.00001100  
H -6.77575100 -3.70571600 -2.35327500  
H -6.77996300 -1.84865200 -3.96605800