

Electronic supplementary information

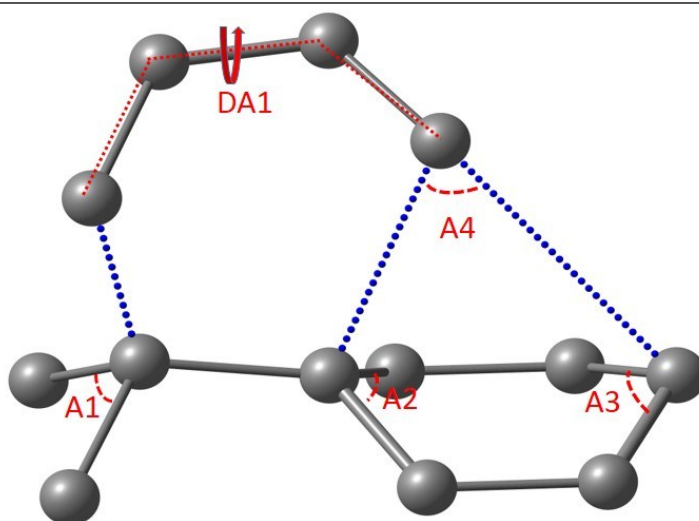
Prediction of [4+2]- and [5+4]-Cycloaddition reaction in Zig-Zag Carbon Nanotubes *Via* Ambimodal Transition State: A Density Functional Theory Calculations.

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Table S1. Important Geometrical Parameters (Bond angle and dihedral angle)



System	Bond Angle				Dihedral angle
	A1	A2	A3	A4	DA1
Butadiene					-32.88
(5,0)CNT	111.06	111.06	114.50		
(6,0)CNT	114.18	114.18	115.07		
(7,0)CNT	117.03	114.40	115.65		
(8,0)CNT	116.69	116.69	117.90		
(5,0)CNT -TS	95.15	103.18	104.61	65.50	-3.29
(6,0)CNT -TS	100.52	107.39	108.12	62.63	3.95
(7,0)CNT -TS	101.17	107.38	110.25	60.07	5.22
(8,0)CNT -TS	101.42	108.51	111.77	61.48	-3.98

All the angles are in degree

Table S2. Geometrical index (l_{x-y}) as defined by Radomir Jasinski.

System	[4+2]Cycloaddition			[5+4]Cycloaddition		
	r_{x-y}^{TS}	r_{x-y}^P	l_{x-y}	r_{x-y}^{TS}	r_{x-y}^P	l_{x-y}
(5,0)CNT	2.53	1.60	0.42	2.35	1.56	0.49
(6,0)CNT	2.82	1.61	0.25	2.38	1.57	0.48
(7,0)CNT	2.99	1.60	0.13	2.35	1.57	0.50
(8,0)CNT	3.01	1.60	0.12	2.49	1.57	0.41

All the distances are in Å

Table S3. Calculated energetics of various cycloaddition reactions.

System	TSs			[4+2]Cycloaddition			[5+4]Cycloaddition		
	ΔE^\ddagger	ΔH^\ddagger	ΔG^\ddagger	ΔE_r	ΔH_r	ΔG_r	ΔH_r	ΔG_r	ΔE_r
(5,0)CNT	-8.29	-5.78	10.85	-52.84	-48.25	-31.34	-51.43	-46.45	-29.45
(6,0)CNT	10.40	10.99	26.49	-21.90	-19.41	-3.48	-39.79	-36.02	-19.76
(7,0)CNT	21.73	22.35	38.27	-9.54	-6.84	9.89	-23.62	-19.94	-2.85
(8,0)CNT	35.64	35.59	50.64	7.61	9.46	25.01	-16.21	-13.02	2.89

All the energies are in kcal/mol.

Table S4. Calculated energetics of various cycloaddition reaction of (5,0)CNT of different length with 1,3-butadiene.

Tube length in (Å)	TSs			[4+2]Cycloaddition			[5+4]Cycloaddition		
	ΔE^\ddagger	ΔH^\ddagger	ΔG^\ddagger	ΔE_r	ΔH_r	ΔG_r	ΔE_r	ΔH_r	ΔG_r
9.25	-8.29	-5.78	10.85	-52.84	-48.25	-31.34	-51.43	-46.45	-29.45
11.34	-4.10	-2.22	14.35	-46.23	-42.23	-25.39	-48.28	-43.86	-26.84
13.49	-3.31	-0.82	16.45	-43.96	-39.33	-21.80	-47.53	-42.37	-24.65
15.63	4.46	7.37	24.64	-35.21	-30.16	-12.57	-40.18	-34.46	-16.55

All the energies are in kcal/mol.

Table S5. Energetics obtained in gas-phase and using different solvents.

System	TS			[4+2]Cycloaddition			[5+4]Cycloaddition		
	ΔE^\ddagger	ΔH^\ddagger	ΔG^\ddagger	ΔE_r	ΔH_r	ΔG_r	ΔE_r	ΔH_r	ΔG_r
(5,0)CNT of 9.25 Å length									
A	-8.29	-5.78	10.85	-52.84	-48.25	-31.34	-51.43	-46.45	-29.45
B	-6.56	-3.92	12.83	-51.26	-46.58	-29.57	-49.69	-44.55	-27.40
C	-6.99	-3.59	12.12	-51.67	-46.16	-30.06	-49.37	-43.37	-27.13
(6,0)CNT of 9.25 Å length									
A	10.40	10.99	26.49	-21.90	-19.41	-3.48	-39.79	-36.02	-19.76
B	10.63	11.57	27.22	-21.51	-18.71	-2.57	-39.00	-34.82	-18.27
C	6.51	8.11	24.83	-24.81	-21.47	-4.30	-40.77	-36.01	-18.40
(5,0)CNT of 11.34 Å length									
A	-4.10	-2.22	14.35	-46.23	-42.23	-25.39	-48.28	-43.86	-26.84
B	-1.48	0.32	16.87	-43.77	-39.88	-23.08	-45.64	-41.29	-24.32
C	-0.97	0.82	16.81	-43.16	-39.12	-22.75	-44.20	-39.84	-23.31

All the energies are in kcal/mol

A are in gas-phase

B are in Toluene solvent

C are in Acetonitrile solvent

Periodic calculations:

The nanotube super cells were constructed from the B3LYP-D3 optimized geometries. The new super-cells were re-optimized using DFT with generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) method. An ultra-soft pseudo-potential description of the electron-electron interaction was used with valence electrons $2s^2, 2p^4$ and $1s^1$ of C and H atoms, respectively. A 50 Ry wave function and a 250 Ry charge density cut-off were taken into account. One-dimensional (1-D) periodic boundary conditions (PBCs) were applied along with the tube axis (Y-axis) to simulate infinitely long alternating nanotube systems. The minimum distance kept between periodic images (in x, and z-axis) is $\sim 20 \text{ \AA}$ to minimize the interactions between periodic images. A Brillouin zone sampling was considered on a Gamma centred $1 \times 8 \times 1$ grid. Geometry optimization was performed to relax both ions and lattices until the total energy variation was less than 10^{-6} eV . All these calculations were performed using Quantum espresso program package.¹

Periodic calculations

The periodic calculations were performed to explore the stability of [4+2] and [5+4] products. Periodic structure analysis clearly indicates the formation of [4+2] cycloadduct is more favourable when compared with corresponding [5+4] counterpart. Typically, calculated energy difference ($\Delta E = E_{[5+4]} - E_{[4+2]}$) for (6,0)CNT is 113.07 kcal/mol. Therefore, it is interesting to mention that the terminal carbon reactivity plays vital role in the formation of [5+4] cyclic adducts.

¹P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, et al. J.Phys.:Condens.Matter 21, 395502 (2009) <http://dx.doi.org/10.1088/0953-8984/21/39/395502>

Role of basis set

To understand the role of single basis set vs multiple basis set, in the present investigation the calculations were performed using B3LYP-D3/6-31+G* and B3LYP-D3/6-311++G** level of theories. The geometries of various point structure change only marginally when compared both above mentioned methods. Calculated energetics of cycloaddition reaction of (7,0)CNT with butadiene using above mentioned methods are depicted in Figure S3.

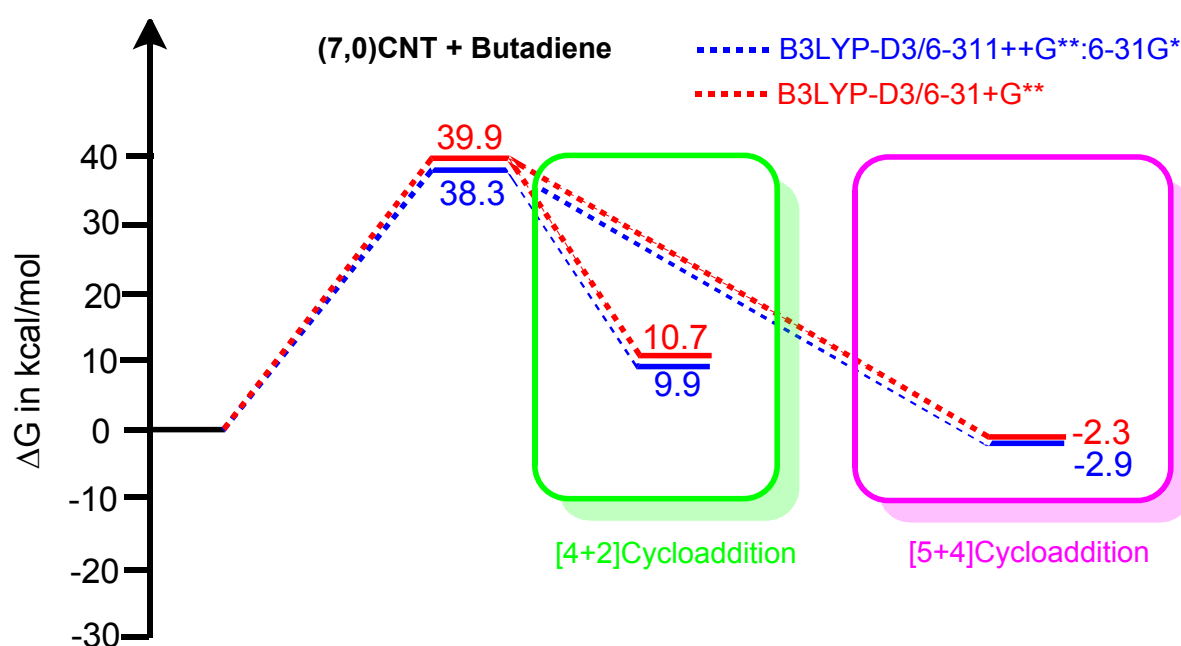


Figure S1. Relative energy profile of (7,0)CNT with 1,3-butadiene using B3LYP-D3 method employing 6-31+G** and 6-311++G**:⁶-31G* basis sets.

It can be noted that energetics of TS and both products change marginally. Typically calculated $\Delta\Delta G_{TS}$ (ΔG_{TS} B3LYP-D3/6-311++G**:⁶-31G* - ΔG_{TS} B3LYP-D3/6-31+G*), $\Delta\Delta G_{[4+2]}$ ($\Delta G_{[4+2]}$ B3LYP-D3/6-311++G**:⁶-31G* - $\Delta G_{[4+2]}$ B3LYP-D3/6-31+G*) and $\Delta\Delta G_{[5+4]}$ ($\Delta G_{[5+4]}$ B3LYP-D3/6-311++G**:⁶-31G* - $\Delta G_{[5+4]}$ B3LYP-D3/6-31+G*) is 1.6, 0.8, and 0.6 kcal, respectively. It is interesting to note that change in the energies obtained from different level of theory for products ([4+2] and [5+4]) is comparable with kT value. Therefore, in the present investigation B3LYP-D3/6-311++G**:⁶-31G* level of theory utilized for all other calculations.

Biradical formation

With reference to **scheme 2** of Text, biradical formation is unavoidable situation in during [5+4]-cycloaddition reaction. Although it is not shown in the case of [4+2] cycloaddition the same intermediate formation can be assumed. Therefore, the unrestricted calculations were also performed using UB3LYP-D3, U ω B97XD and UM06-2X level of theory. Calculated free energy profiles using different methods considering both singlet and triplet transition states and products are given here.

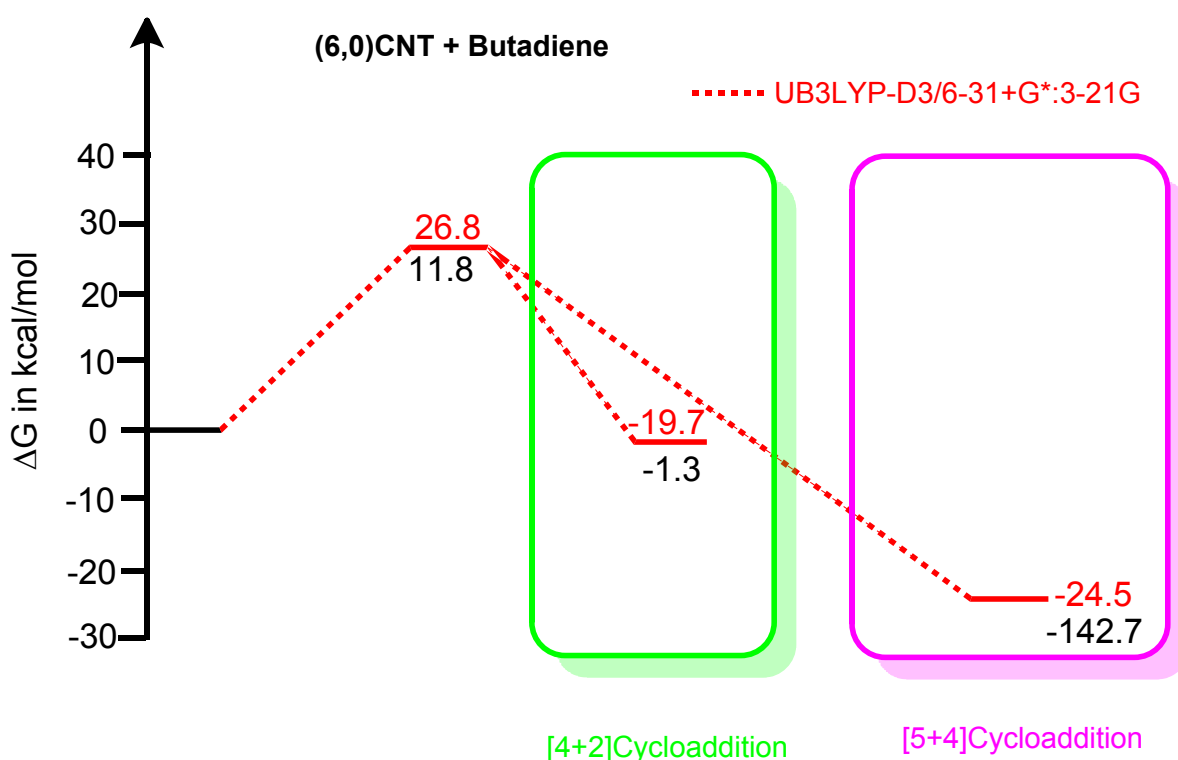


Figure S2. Relative energy profile of (6,0)CNT with 1,3-butadiene using UB3LYP-D3 method employing 6-31+G*:3-21G* basis sets (The values given in red and black color are obtained by considering corresponding state as singlet and triplet).

It is interesting to observe that the stability of triplet ambimodal transition state is more when compared with the singlet counterpart. Further, it can also be noted from the above figure that the singlet [4+2]-cycloadduct is more stable when compared with the stability of triplet [4+2]-cyclic adduct. The [5+4]-cyclic adduct energetically more stable one and significant stability attained in its triplet ground state. The energy difference of singlet and triplet [5+4]-cycloadduct is 118.2 kcal/mol. thus DFT based calculation indicates the [5+4]-cycloadduct is a biradical with triplet ground state.

IRC calculations

As it can be seen from the geometries of various reactant, transition structures and products that change in basis set and inclusion of dispersion in B3LYP influences only marginally. Therefore, the intrinsic reaction coordination calculation carried out using B3LYP-D3/6-31G* level of calculation. Calculated IRC plots are shown in Figure S3.

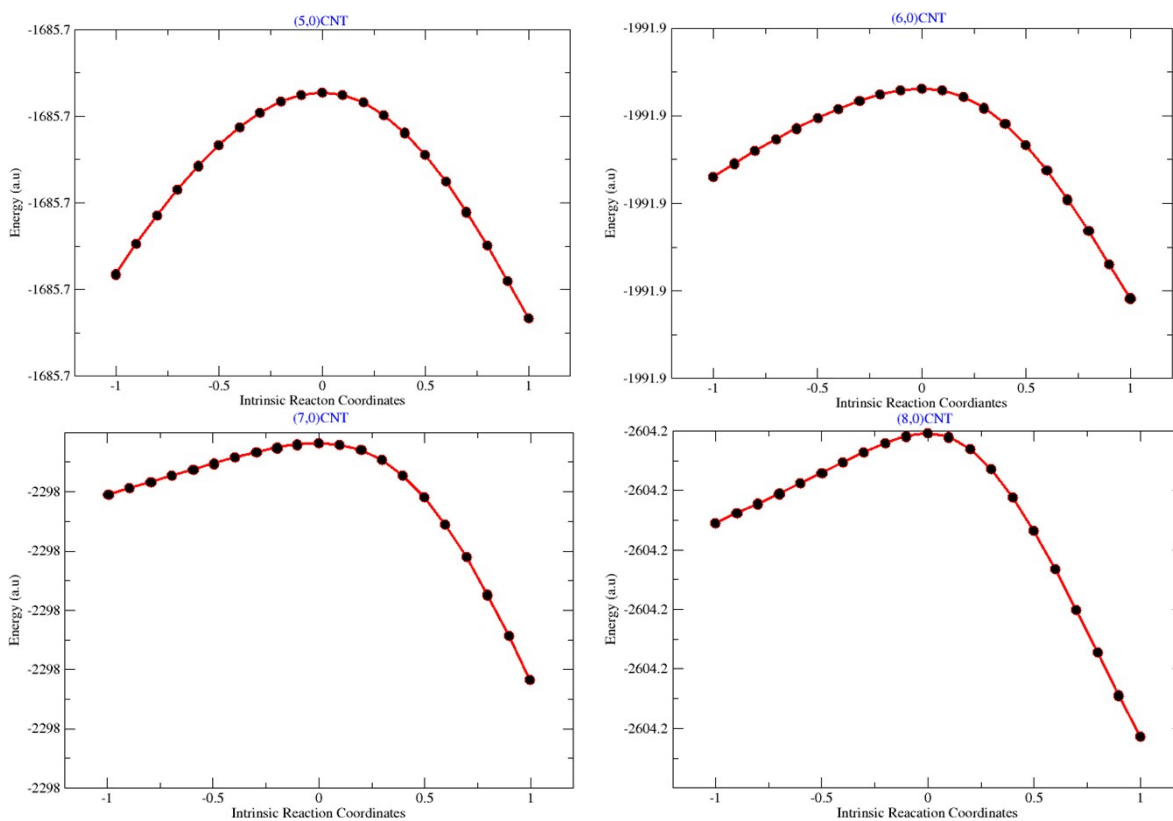


Figure S3. Intrinsic reaction coordinates obtained using various transition structure (Calculations were carried out using B3LYP-D3/6-31G* level of calculations).

PES

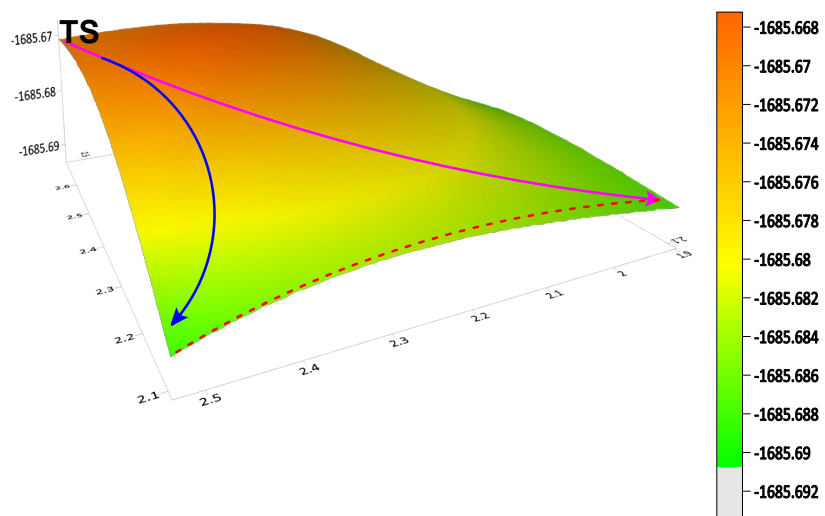


Figure S4. Potential energy surface bifurcation.

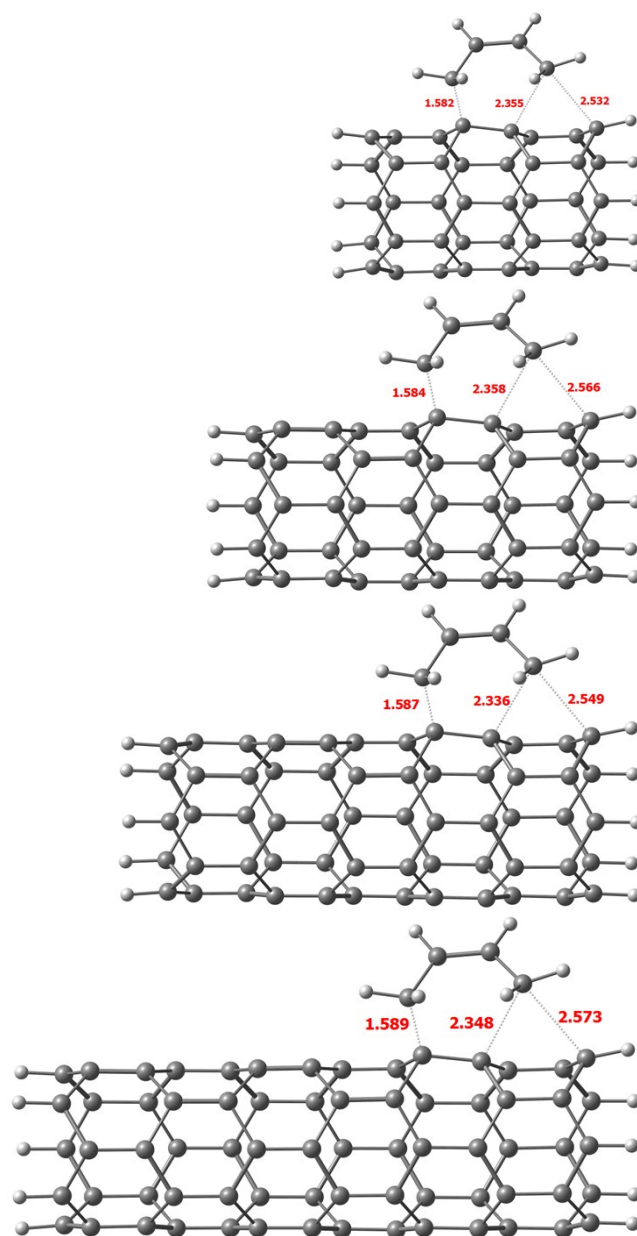


Figure S5. Optimized geometries of TSs involved in DA reaction of different length (5,0)CNT with 1,3-butadiene. (colour key: Gary = Carbon and White = Hydrogen atoms).

The results given here are calculated using B3LYP-D3 employing combined 6-311++G** and 6-31G* basis sets. Further, the all these were optimized with singlet ground state configuration.

Optimized Geometries of pristine tubes with tube length 9.5 Å

(5,0)CNT

6	-1.144578000	3.540990000	1.636281000
6	0.000000000	2.826646000	2.117703000
6	-1.200557000	0.698721000	1.696811000
6	0.000000000	1.413792000	2.126816000
6	-1.200557000	-0.698721000	1.696811000
6	0.000000000	-1.413792000	2.126816000
6	-1.144578000	-3.540990000	1.636281000
6	0.000000000	-2.826646000	2.117703000
6	-1.859059000	3.546674000	-0.627364000
6	-1.890144000	2.854857000	0.616930000
6	-1.906962000	0.707968000	-0.607365000
6	-1.890474000	1.423544000	0.632806000
6	-1.906962000	-0.707968000	-0.607365000
6	-1.890474000	-1.423544000	0.632806000
6	-1.859059000	-3.546674000	-0.627364000
6	-1.890144000	-2.854857000	0.616930000
6	0.000000000	3.534129000	-2.148230000
6	-1.175737000	2.854679000	-1.672582000
6	0.000000000	0.701571000	-2.069894000
6	-1.175576000	1.429910000	-1.639443000
6	0.000000000	-0.701571000	-2.069894000
6	-1.175576000	-1.429910000	-1.639443000
6	0.000000000	-3.534129000	-2.148230000
6	-1.175737000	-2.854679000	-1.672582000
6	1.859059000	3.546674000	-0.627364000
6	1.175737000	2.854679000	-1.672582000
6	1.906962000	0.707968000	-0.607365000
6	1.175576000	1.429910000	-1.639443000
6	1.906962000	-0.707968000	-0.607365000
6	1.175576000	-1.429910000	-1.639443000
6	1.859059000	-3.546674000	-0.627364000
6	1.175737000	-2.854679000	-1.672582000
6	1.144578000	3.540990000	1.636281000
6	1.890144000	2.854857000	0.616930000
6	1.200557000	0.698721000	1.696811000
6	1.890474000	1.423544000	0.632806000
6	1.200557000	-0.698721000	1.696811000
6	1.890474000	-1.423544000	0.632806000
6	1.144578000	-3.540990000	1.636281000
6	1.890144000	-2.854857000	0.616930000
1	-1.178156000	4.625637000	1.694235000

1	1.178156000	4.625637000	1.694235000
1	-1.848620000	4.633346000	-0.626798000
1	1.848620000	4.633346000	-0.626798000
1	0.000000000	4.618131000	-2.159330000
1	-1.178156000	-4.625637000	1.694235000
1	1.178156000	-4.625637000	1.694235000
1	-1.848620000	-4.633346000	-0.626798000
1	1.848620000	-4.633346000	-0.626798000
1	0.000000000	-4.618131000	-2.159330000

Zero-point correction= 0.345391 (Hartree/Particle)
 Thermal correction to Energy= 0.364905
 Thermal correction to Enthalpy= 0.365849
 Thermal correction to Gibbs Free Energy= 0.302310
 Sum of electronic and zero-point Energies= -1529.513374
 Sum of electronic and thermal Energies= -1529.493861
 Sum of electronic and thermal Enthalpies= -1529.492917
Sum of electronic and thermal Free Energies= -1529.556455
Number of imaginary frequencies = 0

(6,0)CNT

6	3.550345000	-0.424005000	-2.381806000
6	2.868132000	0.816254000	-2.257232000
6	0.716783000	-0.421887000	-2.363627000
6	1.425257000	0.816781000	-2.261333000
6	-0.719019000	-0.421889000	-2.363637000
6	-1.427489000	0.816786000	-2.261347000
6	-3.552599000	-0.423989000	-2.381720000
6	-2.870358000	0.816264000	-2.257262000
6	3.550305000	-2.275228000	-0.822852000
6	2.868308000	-1.544550000	-1.833264000
6	0.716772000	-2.255770000	-0.815853000
6	1.425467000	-1.547687000	-1.836887000
6	-0.719010000	-2.255777000	-0.815856000
6	-1.427700000	-1.547696000	-1.836899000
6	-3.552561000	-2.275130000	-0.822817000
6	-2.870534000	-1.544569000	-1.833291000
6	3.550412000	-1.849468000	1.559536000
6	2.868360000	-2.360830000	0.421397000
6	0.716808000	-1.836152000	1.546645000
6	1.425526000	-2.365528000	0.422099000
6	-0.719045000	-1.836159000	1.546652000
6	-1.427759000	-2.365539000	0.422101000
6	-3.552668000	-1.849400000	1.559480000
6	-2.870588000	-2.360856000	0.421403000
6	3.547692000	0.427638000	2.383379000
6	2.868129000	-0.816783000	2.257063000
6	0.717098000	0.420405000	2.362347000
6	1.425255000	-0.819053000	2.260520000
6	-0.719334000	0.420407000	2.362356000

6	-1.427486000	-0.819058000	2.260533000
6	-3.549945000	0.427617000	2.383285000
6	-2.870355000	-0.816793000	2.257093000
6	3.544435000	2.275467000	0.822941000
6	2.865087000	1.543131000	1.831530000
6	0.716040000	2.250208000	0.813806000
6	1.423647000	1.542612000	1.832616000
6	-0.718276000	2.250219000	0.813811000
6	-1.425879000	1.542619000	1.832626000
6	-3.546689000	2.275374000	0.822908000
6	-2.867311000	1.543147000	1.831551000
6	3.547792000	1.853224000	-1.558392000
6	2.865154000	2.358700000	-0.421001000
6	0.717119000	1.834194000	-1.546638000
6	1.423707000	2.359016000	-0.422144000
6	-0.719355000	1.834201000	-1.546643000
6	-1.425939000	2.359025000	-0.422145000
6	-3.550047000	1.853147000	-1.558332000
6	-2.867379000	2.358721000	-0.421004000
1	4.637365000	-1.823942000	1.538771000
1	4.637229000	-2.243938000	-0.811650000
1	4.634795000	0.425997000	2.349856000
1	4.637345000	-0.417751000	-2.350476000
1	4.628995000	2.249206000	0.813576000
1	4.634840000	1.829743000	-1.532927000
1	-4.639619000	-1.823917000	1.538754000
1	-4.639483000	-2.243897000	-0.811637000
1	-4.637047000	0.425989000	2.349821000
1	-4.639598000	-0.417744000	-2.350444000
1	-4.631248000	2.249176000	0.813568000
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Zero-point correction= 0.422345 (Hartree/Particle)
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 Sum of electronic and thermal Energies= -1835.644142
 Sum of electronic and thermal Enthalpies= -1835.643197
Sum of electronic and thermal Free Energies= -1835.712462
Number of imaginary frequencies = 0

(7,0)CNT

1	4.670160000	1.722591000	2.159847000
6	2.927197000	2.486948000	1.153187000
6	3.584602000	1.774288000	2.195668000
6	1.482059000	2.489884000	1.140284000
6	0.750513000	1.760204000	2.128039000
6	-1.371825000	2.593280000	1.161817000
6	-0.678200000	1.797490000	2.133113000

6	-2.809549000	2.581894000	1.168132000
6	-3.512080000	1.820247000	2.145529000
1	-4.599666000	1.821896000	2.123820000
1	4.684949000	2.741586000	-0.061228000
6	2.916434000	2.439234000	-1.248520000
6	3.599236000	2.797828000	-0.056584000
6	1.469928000	2.444290000	-1.262097000
6	0.762491000	2.767544000	-0.066385000
6	-1.378117000	2.547569000	-1.275266000
6	-0.667153000	2.807435000	-0.060346000
6	-2.813970000	2.537685000	-1.259667000
6	-3.499584000	2.797896000	-0.047370000
1	-4.587315000	2.779427000	-0.044630000
1	4.661853000	1.619162000	-2.215856000
6	2.866656000	0.529894000	-2.726459000
6	3.575461000	1.659927000	-2.230614000
6	1.423649000	0.534807000	-2.742598000
6	0.736963000	1.673673000	-2.219812000
6	-1.420452000	0.599322000	-2.732662000
6	-0.691395000	1.713810000	-2.214347000
6	-2.863105000	0.598048000	-2.716063000
6	-3.526216000	1.724119000	-2.182149000
1	-4.613483000	1.728096000	-2.151248000
1	4.616214000	-0.731830000	-2.654972000
6	2.816156000	-1.827827000	-2.157284000
6	3.528994000	-0.715757000	-2.682898000
6	1.379927000	-1.830723000	-2.175805000
6	0.693893000	-0.693150000	-2.708900000
6	-1.467956000	-1.741130000	-2.127684000
6	-0.734558000	-0.653696000	-2.700276000
6	-2.914507000	-1.740989000	-2.113098000
6	-3.573013000	-0.635189000	-2.703851000
1	-4.659456000	-0.603159000	-2.675801000
1	4.587677000	-2.535163000	-1.137910000
6	2.808147000	-2.837623000	0.051041000
6	3.499918000	-2.549908000	-1.148901000
6	1.370929000	-2.845548000	0.040594000
6	0.667650000	-2.552700000	-1.166415000
6	-1.482806000	-2.739030000	0.058625000
6	-0.762095000	-2.512896000	-1.158114000
6	-2.927876000	-2.740592000	0.071899000
6	-3.599056000	-2.541975000	-1.161779000
1	-4.684853000	-2.489617000	-1.145459000
1	4.597762000	-2.517763000	1.231521000
6	2.844934000	-1.720718000	2.201317000
6	3.510131000	-2.524118000	1.250386000
6	1.400670000	-1.721710000	2.190740000
6	0.676586000	-2.499856000	1.247753000
6	-1.451925000	-1.647569000	2.195105000
6	-0.752236000	-2.462928000	1.255971000

6	-2.898176000	-1.651968000	2.208510000
6	-3.586176000	-2.502322000	1.311601000
1	-4.671774000	-2.441565000	1.298916000
1	4.629012000	-0.639175000	2.732079000
6	2.895659000	0.638419000	2.681765000
6	3.544667000	-0.620766000	2.761266000
6	1.449263000	0.639135000	2.667994000
6	0.711151000	-0.580092000	2.705896000
6	-1.403311000	0.708962000	2.689031000
6	-0.713590000	-0.542578000	2.712744000
6	-2.847909000	0.704146000	2.699221000
6	-3.546991000	-0.527311000	2.781935000
1	-4.631306000	-0.498327000	2.761618000

Zero-point correction= 0.493216 (Hartree/Particle)
 Thermal correction to Energy= 0.521140
 Thermal correction to Enthalpy= 0.522084
 Thermal correction to Gibbs Free Energy= 0.442953
 Sum of electronic and zero-point Energies= -2141.773530
 Sum of electronic and thermal Energies= -2141.745605
 Sum of electronic and thermal Enthalpies= -2141.744661
Sum of electronic and thermal Free Energies= -2141.823793
Number of imaginary frequencies = 0

(8,0)CNT

6	1.219547000	2.943654000	3.551003000
6	0.000473000	3.163429000	2.872154000
6	1.207547000	2.914764000	0.718732000
6	-0.000420000	3.159445000	1.426171000
6	1.207547000	2.914764000	-0.718732000
6	-0.000420000	3.159445000	-1.426171000
6	1.219547000	2.943654000	-3.551003000
6	0.000473000	3.163429000	-2.872154000
6	2.942525000	1.222370000	3.554811000
6	2.237707000	2.238197000	2.872156000
6	2.920622000	1.210213000	0.719619000
6	2.235478000	2.234719000	1.426049000
6	2.920622000	1.210213000	-0.719619000
6	2.235478000	2.234719000	-1.426049000
6	2.942525000	1.222370000	-3.554811000
6	2.237707000	2.238197000	-2.872156000
6	2.942635000	-1.218160000	3.557147000
6	3.167276000	0.000321000	2.875224000
6	2.921706000	-1.210395000	0.719460000
6	3.166830000	-0.000310000	1.427807000
6	2.921706000	-1.210395000	-0.719460000
6	3.166830000	-0.000310000	-1.427807000
6	2.942635000	-1.218160000	-3.557147000
6	3.167276000	0.000321000	-2.875224000
6	1.218856000	-2.943084000	3.556836000

6	2.238448000	-2.238540000	2.875400000
6	1.209783000	-2.920618000	0.719360000
6	2.238744000	-2.238721000	1.427951000
6	1.209783000	-2.920618000	-0.719360000
6	2.238744000	-2.238721000	-1.427951000
6	1.218856000	-2.943084000	-3.556836000
6	2.238448000	-2.238540000	-2.875400000
6	-1.219863000	-2.944679000	3.556543000
6	-0.000382000	-3.166396000	2.875049000
6	-1.210154000	-2.921233000	0.719262000
6	-0.000167000	-3.165685000	1.427832000
6	-1.210154000	-2.921233000	-0.719262000
6	-0.000167000	-3.165685000	-1.427832000
6	-1.219863000	-2.944679000	-3.556543000
6	-0.000382000	-3.166396000	-2.875049000
6	-2.943035000	-1.219394000	3.556840000
6	-2.239554000	-2.239971000	2.875090000
6	-2.920737000	-1.209925000	0.719362000
6	-2.239200000	-2.239315000	1.427747000
6	-2.920737000	-1.209925000	-0.719362000
6	-2.239200000	-2.239315000	-1.427747000
6	-2.943035000	-1.219394000	-3.556840000
6	-2.239554000	-2.239971000	-2.875090000
6	-2.942347000	1.219521000	3.557121000
6	-3.164967000	-0.000123000	2.875358000
6	-2.922005000	1.210187000	0.719458000
6	-3.165302000	-0.000042000	1.428041000
6	-2.922005000	1.210187000	-0.719458000
6	-3.165302000	-0.000042000	-1.428041000
6	-2.942347000	1.219521000	-3.557121000
6	-3.164967000	-0.000123000	-2.875358000
6	-1.216377000	2.944439000	3.554840000
6	-2.240140000	2.240383000	2.875249000
6	-1.209474000	2.920444000	0.719619000
6	-2.240256000	2.239624000	1.427702000
6	-1.209474000	2.920444000	-0.719619000
6	-2.240256000	2.239624000	-1.427702000
6	-1.216377000	2.944439000	-3.554840000
6	-2.240140000	2.240383000	-2.875249000
1	1.209169000	-2.919832000	-4.643953000
1	2.920131000	-1.208275000	-4.644356000
1	-1.210040000	-2.921090000	-4.643642000
1	2.916407000	1.216233000	-4.642232000
1	-2.919786000	-1.209753000	-4.643957000
1	1.212098000	2.925398000	-4.635931000
1	-2.919366000	1.210566000	-4.644331000
1	-1.202406000	2.921638000	-4.642257000
1	1.209169000	-2.919832000	4.643953000
1	2.920131000	-1.208275000	4.644356000
1	-1.210040000	-2.921090000	4.643642000

1	2.916407000	1.216233000	4.642232000
1	-2.919786000	-1.209753000	4.643957000
1	1.212098000	2.925398000	4.635931000
1	-2.919366000	1.210566000	4.644331000
1	-1.202406000	2.921638000	4.642257000

Zero-point correction= 0.569700 (Hartree/Particle)
 Thermal correction to Energy= 0.600629
 Thermal correction to Enthalpy= 0.601573
 Thermal correction to Gibbs Free Energy= 0.517732
 Sum of electronic and zero-point Energies= -2447.903085
 Sum of electronic and thermal Energies= -2447.872156
 Sum of electronic and thermal Enthalpies= -2447.871211
Sum of electronic and thermal Free Energies= -2447.955053
Number of imaginary frequencies = 0

Optimized Geometries of TSs tubes with tube length 9.5 Å

(5,0)CNT_{TS}

6	3.149435000	-2.710327000	0.963031000
6	2.376187000	-3.071465000	-0.200796000
6	0.316136000	-2.449612000	1.052545000
6	0.989710000	-2.863450000	-0.196207000
6	-1.051132000	-2.257823000	1.045254000
6	-1.818705000	-2.539424000	-0.196639000
6	-3.862249000	-1.797331000	0.940815000
6	-3.194457000	-2.380863000	-0.198113000
6	3.451795000	-0.496982000	1.769145000
6	2.595109000	-1.652376000	1.743687000
6	0.643219000	-0.153784000	1.784503000
6	1.182088000	-1.477667000	1.725991000
6	-0.751703000	0.058520000	1.751366000
6	-1.627834000	-1.074755000	1.676920000
6	-3.526638000	0.455854000	1.772330000
6	-3.037062000	-0.874547000	1.688712000
6	3.614276000	1.409980000	0.213181000
6	2.920846000	0.716459000	1.315398000
6	0.982890000	1.703962000	0.224809000
6	1.514519000	0.875019000	1.293423000
6	-0.475198000	2.104194000	0.233715000
6	-1.278048000	1.319306000	1.308868000
6	-3.317792000	2.134057000	0.208114000
6	-2.672886000	1.506774000	1.343909000
6	3.486859000	-0.184778000	-1.656244000
6	2.944685000	0.930594000	-1.006738000
6	0.682548000	0.162641000	-1.655803000
6	1.541673000	1.094282000	-0.978854000
6	-0.714728000	0.362514000	-1.621951000
6	-1.254413000	1.520175000	-0.976122000
6	-3.489399000	0.759166000	-1.636329000

6	-2.648764000	1.715020000	-1.008169000
6	3.173305000	-2.506989000	-1.263928000
6	2.633162000	-1.324164000	-1.850508000
6	0.342414000	-2.229010000	-1.362841000
6	1.220701000	-1.151005000	-1.828500000
6	-1.024654000	-2.042484000	-1.352183000
6	-1.589271000	-0.765060000	-1.774597000
6	-3.837443000	-1.605296000	-1.231944000
6	-2.997885000	-0.564833000	-1.784406000
1	4.213826000	-2.925301000	1.007484000
1	4.238743000	-2.712693000	-1.324567000
1	4.529948000	-0.645033000	1.760396000
1	4.565066000	-0.332611000	-1.651124000
1	4.696113000	1.509182000	0.234928000
1	-4.943802000	-1.791457000	1.035923000
1	-4.916391000	-1.582650000	-1.350722000
1	-4.601190000	0.623706000	1.791765000
1	-4.564025000	0.927600000	-1.645983000
1	-4.361796000	2.421466000	0.223060000
6	1.626372000	4.294768000	-0.587100000
6	0.277106000	4.377113000	-0.634517000
1	2.201213000	4.739508000	-1.395699000
1	-0.202016000	4.896593000	-1.457069000
6	2.363449000	3.598540000	0.448032000
1	3.428904000	3.786472000	0.447854000
1	1.953718000	3.591767000	1.451456000
6	-0.581924000	3.676830000	0.366886000
1	-1.624907000	3.976830000	0.272376000
1	-0.271196000	3.906169000	1.391056000

Zero-point correction= 0.436457 (Hartree/Particle)
 Thermal correction to Energy= 0.459221
 Thermal correction to Enthalpy= 0.460165
 Thermal correction to Gibbs Free Energy= 0.390878
 Sum of electronic and zero-point Energies= -1685.474591
 Sum of electronic and thermal Energies= -1685.451827
 Sum of electronic and thermal Enthalpies= -1685.450883
Sum of electronic and thermal Free Energies= -1685.520171
Number of imaginary frequencies = 1 (-461.7724)

(6,0)CNT_{TS}

6	-3.786937000	-0.908707000	2.020346000
6	-2.905236000	0.183029000	2.191542000
6	-0.995441000	-1.384619000	2.047709000
6	-1.482756000	-0.053475000	2.185561000
6	0.426473000	-1.621973000	2.059548000
6	1.319846000	-0.519476000	2.224735000
6	3.221321000	-2.065078000	2.056591000
6	2.743052000	-0.751939000	2.237318000
6	-4.037404000	-2.407598000	0.201298000

6	-3.274915000	-2.048039000	1.352633000
6	-1.230238000	-2.902316000	0.205993000
6	-1.855808000	-2.289560000	1.360633000
6	0.164761000	-3.126827000	0.206945000
6	0.950178000	-2.749141000	1.364978000
6	2.987154000	-3.504037000	0.202632000
6	2.369523000	-2.972686000	1.365815000
6	-3.835250000	-1.220182000	-1.839438000
6	-3.304083000	-2.239053000	-1.011705000
6	-1.043507000	-1.702289000	-1.862049000
6	-1.885481000	-2.482821000	-1.016607000
6	0.377627000	-1.942967000	-1.871580000
6	0.920840000	-2.943282000	-1.015920000
6	3.173750000	-2.384417000	-1.863934000
6	2.339800000	-3.167890000	-1.015823000
6	-3.419716000	1.161048000	-2.013507000
6	-2.960024000	-0.172346000	-2.205900000
6	-0.641769000	0.681556000	-1.990602000
6	-1.537039000	-0.408824000	-2.198013000
6	0.772028000	0.435985000	-2.017074000
6	1.265296000	-0.883910000	-2.235015000
6	3.572076000	-0.012265000	-2.006890000
6	2.689628000	-1.116181000	-2.239815000
6	-3.180479000	2.645295000	-0.219745000
6	-2.541572000	2.072163000	-1.380825000
6	-0.338323000	2.542903000	-0.244687000
6	-1.146604000	1.859258000	-1.376849000
6	1.116917000	2.106934000	-0.235086000
6	1.646124000	1.339111000	-1.353977000
6	3.801699000	1.634526000	-0.219997000
6	3.053418000	1.106054000	-1.351700000
6	-3.372973000	1.468115000	1.795953000
6	-2.513130000	2.263140000	1.003003000
6	-0.595879000	0.986743000	1.778528000
6	-1.118296000	2.048962000	0.997314000
6	0.819628000	0.748715000	1.804514000
6	1.676272000	1.536682000	0.989656000
6	3.616987000	0.298551000	1.810802000
6	3.080584000	1.297045000	0.995960000
1	-4.904985000	-1.024335000	-1.815767000
1	-5.110741000	-2.234717000	0.200553000
1	-4.488909000	1.362184000	-2.015840000
1	-4.857392000	-0.717085000	1.992602000
1	-4.216913000	2.960478000	-0.232979000
1	-4.442555000	1.667283000	1.789615000
1	4.248283000	-2.553010000	-1.844608000
1	4.060817000	-3.677392000	0.203551000
1	4.644408000	-0.196028000	-1.981519000
1	4.295529000	-2.236082000	2.039564000
1	4.887070000	1.606312000	-0.231046000

1	4.689172000	0.112932000	1.791558000
6	0.369304000	4.838182000	0.647784000
6	1.724225000	4.759163000	0.613147000
1	-0.131925000	5.324761000	1.476891000
1	2.301061000	5.161681000	1.442206000
6	-0.437510000	4.133927000	-0.378558000
1	-1.489963000	4.412957000	-0.320148000
1	-0.101333000	4.361924000	-1.394197000
6	2.425341000	4.083054000	-0.432715000
1	3.504264000	4.105031000	-0.405434000
1	2.013191000	4.073625000	-1.432566000

Zero-point correction= 0.509690 (Hartree/Particle)
 Thermal correction to Energy= 0.536573
 Thermal correction to Enthalpy= 0.537517
 Thermal correction to Gibbs Free Energy= 0.460683
 Sum of electronic and zero-point Energies= -1991.602257
 Sum of electronic and thermal Energies= -1991.575374
 Sum of electronic and thermal Enthalpies= -1991.574430
Sum of electronic and thermal Free Energies= -1991.651264
Number of imaginary frequencies = 1 (-394.4235)

(7,0)CNT_{TS}

1	4.205828000	-2.211056000	-2.219097000
6	2.113914000	-1.908998000	-2.653848000
6	3.404752000	-1.475792000	-2.246626000
6	1.021461000	-0.965539000	-2.611520000
6	1.252663000	0.363653000	-2.153503000
6	-1.131392000	0.914237000	-2.577679000
6	0.167370000	1.315363000	-2.110060000
6	-2.219406000	1.853804000	-2.628354000
6	-1.947949000	3.183883000	-2.225787000
1	-2.773683000	3.890756000	-2.188075000
1	2.625356000	-4.004381000	-2.598316000
6	0.579480000	-3.661175000	-1.999852000
6	1.804621000	-3.291044000	-2.612326000
6	-0.516193000	-2.719301000	-1.985439000
6	-0.329179000	-1.428941000	-2.551428000
6	-2.662919000	-0.831659000	-1.971214000
6	-1.402869000	-0.482034000	-2.537542000
6	-3.756797000	0.113140000	-1.994887000
6	-3.555163000	1.358373000	-2.633140000
1	-4.365427000	2.082842000	-2.611645000
1	1.462062000	-5.344590000	-0.974651000
6	-0.028618000	-4.350140000	0.234031000
6	0.626242000	-4.648957000	-0.987939000
6	-1.128810000	-3.413251000	0.244209000
6	-1.532849000	-2.802803000	-0.978531000
6	-3.270198000	-1.530251000	0.239905000
6	-2.608161000	-1.861897000	-0.977299000

6	-4.366264000	-0.583814000	0.216730000
6	-4.784353000	-0.038042000	-1.020057000
1	-5.582988000	0.699404000	-1.007341000
1	1.602252000	-5.175175000	1.387922000
6	0.798232000	-3.385934000	2.293196000
6	0.765844000	-4.479767000	1.398369000
6	-0.294780000	-2.447560000	2.300950000
6	-1.407874000	-2.651578000	1.421706000
6	-2.432648000	-0.570599000	2.284225000
6	-2.481127000	-1.709629000	1.419509000
6	-3.521511000	0.375220000	2.255350000
6	-4.635212000	0.144682000	1.405882000
1	-5.436697000	0.879182000	1.393409000
1	2.917259000	-3.657603000	2.644723000
6	2.389153000	-1.569190000	2.556248000
6	2.096971000	-2.943122000	2.660907000
6	1.298050000	-0.626701000	2.540595000
6	-0.046359000	-1.093123000	2.665606000
6	-0.832962000	1.243239000	2.521745000
6	-1.120141000	-0.144645000	2.647226000
6	-1.918447000	2.182339000	2.513112000
6	-3.251483000	1.720121000	2.602448000
1	-4.060950000	2.445762000	2.564878000
1	4.429012000	-1.947994000	1.933022000
6	3.617581000	-0.216669000	0.959789000
6	3.624250000	-1.215519000	1.939029000
6	2.536765000	0.745340000	0.964802000
6	1.482838000	0.635004000	1.906498000
6	0.438016000	2.683576000	1.005022000
6	0.401765000	1.589796000	1.882585000
6	-0.651130000	3.596929000	0.991928000
6	-1.711835000	3.447755000	1.898233000
1	-2.534115000	4.160444000	1.872537000
1	5.178127000	-1.107566000	-0.244532000
6	3.486406000	-0.375277000	-1.378269000
6	4.363678000	-0.389400000	-0.248115000
6	2.398454000	0.577950000	-1.359320000
6	2.313508000	1.504039000	-0.244066000
6	0.260051000	2.483298000	-1.354874000
6	1.319609000	2.649397000	-0.252624000
6	-0.838433000	3.410741000	-1.379690000
6	-1.043382000	4.237842000	-0.239356000
1	-1.832428000	4.980893000	-0.235993000
6	4.269024000	3.525893000	0.535101000
6	3.135015000	4.291065000	0.564564000
1	4.949239000	3.557275000	1.382865000
1	2.930641000	4.925498000	1.419821000
6	4.534174000	2.606115000	-0.497928000
1	5.407838000	1.975726000	-0.447314000
1	4.124598000	2.750211000	-1.487074000

6	2.086729000	4.089108000	-0.443819000
1	1.325749000	4.866204000	-0.408950000
1	2.479294000	4.056854000	-1.462617000

Zero-point correction= 0.580753 (Hartree/Particle)
 Thermal correction to Energy= 0.612467
 Thermal correction to Enthalpy= 0.613411
 Thermal correction to Gibbs Free Energy= 0.527379
 Sum of electronic and zero-point Energies= -2297.690447
 Sum of electronic and thermal Energies= -2297.658733
 Sum of electronic and thermal Enthalpies= -2297.657789
Sum of electronic and thermal Free Energies= -2297.743821
Number of imaginary frequencies = 1 (-308.6605)

(8,0)CNT_{TS}

6	3.400540000	3.197091000	-0.223902000
6	2.828693000	2.578229000	-1.381091000
6	3.231172000	0.418744000	-0.244699000
6	2.686547000	1.139154000	-1.383667000
6	3.264698000	-1.111390000	-0.255078000
6	2.425701000	-1.705219000	-1.400511000
6	2.558742000	-3.881711000	-0.236619000
6	2.241926000	-3.123507000	-1.406594000
6	2.358131000	3.294601000	1.990182000
6	2.979585000	2.555800000	0.983063000
6	2.020816000	0.485723000	1.920793000
6	2.842173000	1.117911000	0.974526000
6	1.857156000	-0.957668000	1.889684000
6	2.578843000	-1.728149000	0.976189000
6	1.569374000	-3.759719000	1.936758000
6	2.395590000	-3.145328000	0.979126000
6	0.169943000	3.520569000	3.024712000
6	1.270885000	2.709728000	2.702999000
6	-0.162862000	0.709782000	2.985505000
6	1.104224000	1.277289000	2.671326000
6	-0.323241000	-0.721240000	2.967165000
6	0.784250000	-1.543728000	2.626614000
6	-0.634961000	-3.534571000	2.959921000
6	0.622032000	-2.973481000	2.637453000
6	-2.137225000	3.789136000	2.346234000
6	-1.138031000	2.977854000	2.917860000
6	-2.487869000	0.968153000	2.349709000
6	-1.306387000	1.544348000	2.915516000
6	-2.649697000	-0.456497000	2.345522000
6	-1.621129000	-1.285786000	2.896608000
6	-2.974094000	-3.277696000	2.344470000
6	-1.786120000	-2.720950000	2.880367000
6	-3.252199000	3.923895000	0.215778000
6	-3.014296000	3.199116000	1.404132000

6	-3.613950000	1.101883000	0.212415000
6	-3.194220000	1.763713000	1.406073000
6	-3.777427000	-0.321607000	0.209359000
6	-3.512493000	-1.068212000	1.396693000
6	-4.122513000	-3.141771000	0.204890000
6	-3.676664000	-2.508823000	1.389032000
6	-2.422180000	3.831046000	-2.044171000
6	-3.168409000	3.221826000	-1.006538000
6	-2.772462000	1.010405000	-2.054848000
6	-3.349400000	1.786722000	-1.012164000
6	-2.934218000	-0.414515000	-2.056796000
6	-3.667087000	-1.045391000	-1.016080000
6	-3.260740000	-3.235315000	-2.067889000
6	-3.831653000	-2.485856000	-1.015256000
6	-0.222606000	3.579080000	-3.024455000
6	-1.506442000	3.032716000	-2.756702000
6	-0.551558000	0.767039000	-2.995291000
6	-1.675038000	1.599178000	-2.758896000
6	-0.709107000	-0.664243000	-2.982333000
6	-1.988110000	-1.231802000	-2.754314000
6	-1.021759000	-3.478270000	-2.984829000
6	-2.151158000	-2.667111000	-2.742988000
6	2.082763000	3.335593000	-2.284857000
6	0.909871000	2.764289000	-2.861998000
6	1.751105000	0.524322000	-2.232190000
6	0.746028000	1.330585000	-2.838309000
6	1.592972000	-0.918399000	-2.202299000
6	0.431698000	-1.492355000	-2.802402000
6	1.296411000	-3.720040000	-2.260837000
6	0.267589000	-2.922062000	-2.816992000
1	-3.078346000	-4.359903000	2.322910000
1	-0.749565000	-4.616005000	2.933689000
1	-4.216985000	-4.225013000	0.200703000
1	1.445260000	-4.840737000	1.912089000
1	-3.363792000	-4.317783000	-2.054648000
1	2.491823000	-4.963423000	-0.242541000
1	-1.133531000	-4.560083000	-2.962409000
1	1.174923000	-4.801403000	-2.240399000
1	-1.998590000	4.867841000	2.331730000
1	0.290188000	4.601820000	3.017972000
1	-3.100046000	5.000756000	0.216248000
1	2.458303000	4.378318000	1.988834000
1	-2.282106000	4.909517000	-2.027457000
1	3.549921000	4.272298000	-0.223889000
1	-0.101710000	4.660187000	-3.012701000
1	2.181744000	4.419295000	-2.272899000
6	5.948007000	0.223874000	0.647067000
6	5.659098000	-1.104011000	0.672391000
1	6.458907000	0.681256000	1.490538000
1	5.962060000	-1.722519000	1.509680000

6	5.483909000	1.059881000	-0.405666000
1	5.684195000	2.118779000	-0.357029000
1	5.397436000	0.665357000	-1.408453000
6	4.772438000	-1.663107000	-0.371752000
1	5.103602000	-1.396034000	-1.379700000
1	4.732684000	-2.750968000	-0.324971000

Zero-point correction= 0.655652 (Hartree/Particle)
 Thermal correction to Energy= 0.690878
 Thermal correction to Enthalpy= 0.691822
 Thermal correction to Gibbs Free Energy= 0.599691
 Sum of electronic and zero-point Energies= -2603.799409
 Sum of electronic and thermal Energies= -2603.764183
 Sum of electronic and thermal Enthalpies= -2603.763239
Sum of electronic and thermal Free Energies= -2603.855370
Number of imaginary frequencies = 1 (-433.5613)

Optimized Geometries of [4+2] Adduct tubes with tube length 9.5 Å

(5,0) Adduct

6	3.528143000	-2.290842000	0.956771000
6	2.804982000	-2.761330000	-0.201120000
6	0.687390000	-2.373231000	1.043227000
6	1.413770000	-2.739959000	-0.199164000
6	-0.687392000	-2.373231000	1.043227000
6	-1.413771000	-2.739961000	-0.199164000
6	-3.528144000	-2.290844000	0.956770000
6	-2.804982000	-2.761334000	-0.201120000
6	3.520532000	-0.038042000	1.793820000
6	2.833943000	-1.279617000	1.704351000
6	0.706881000	-0.015737000	1.696632000
6	1.408588000	-1.263681000	1.657244000
6	-0.706881000	-0.015736000	1.696631000
6	-1.408590000	-1.263680000	1.657242000
6	-3.520533000	-0.038040000	1.793814000
6	-2.833944000	-1.279615000	1.704347000
6	3.584621000	1.636406000	0.204291000
6	2.846021000	1.121072000	1.341360000
6	0.797421000	2.096861000	0.246312000
6	1.431915000	1.153350000	1.287096000
6	-0.797419000	2.096861000	0.246311000
6	-1.431914000	1.153351000	1.287096000
6	-3.584618000	1.636411000	0.204291000
6	-2.846020000	1.121075000	1.341360000
6	3.520162000	0.273560000	-1.664717000
6	2.846690000	1.328573000	-1.006271000
6	0.707473000	0.280066000	-1.562884000
6	1.432374000	1.352402000	-0.945994000
6	-0.707473000	0.280066000	-1.562883000
6	-1.432373000	1.352403000	-0.945994000

6	-3.520162000	0.273561000	-1.664712000
6	-2.846688000	1.328576000	-1.006270000
6	3.527565000	-2.092501000	-1.257584000
6	2.833187000	-0.962064000	-1.809770000
6	0.687207000	-2.158328000	-1.356662000
6	1.408166000	-0.954336000	-1.759306000
6	-0.687208000	-2.158328000	-1.356662000
6	-1.408167000	-0.954335000	-1.759305000
6	-3.527566000	-2.092501000	-1.257581000
6	-2.833188000	-0.962063000	-1.809766000
1	4.606564000	-2.396734000	1.033459000
1	4.605979000	-2.182669000	-1.352507000
1	4.607956000	-0.034557000	1.829350000
1	4.607748000	0.281253000	-1.693932000
1	4.662065000	1.743654000	0.214249000
1	-4.606564000	-2.396738000	1.033459000
1	-4.605981000	-2.182670000	-1.352506000
1	-4.607958000	-0.034554000	1.829345000
1	-4.607748000	0.281256000	-1.693927000
1	-4.662062000	1.743663000	0.214250000
6	0.665374000	4.473357000	-0.611620000
6	-0.665372000	4.473357000	-0.611620000
1	1.257921000	5.072688000	-1.294092000
1	-1.257919000	5.072688000	-1.294093000
6	1.328234000	3.556705000	0.376120000
1	2.411407000	3.573777000	0.269247000
1	1.118385000	3.886443000	1.401426000
6	-1.328233000	3.556705000	0.376120000
1	-2.411406000	3.573777000	0.269246000
1	-1.118385000	3.886443000	1.401426000
Zero-point correction=			0.439977 (Hartree/Particle)
Thermal correction to Energy=			0.462556
Thermal correction to Enthalpy=			0.463500
Thermal correction to Gibbs Free Energy=			0.394636
Sum of electronic and zero-point Energies=			-1685.542075
Sum of electronic and thermal Energies=			-1685.519496
Sum of electronic and thermal Enthalpies=			-1685.518552
Sum of electronic and thermal Free Energies=			-1685.587417
Number of imaginary frequencies = 0			

(6,0) Adduct

6	-3.546774000	-1.528701000	2.021051000
6	-2.857615000	-0.304801000	2.180881000
6	-0.720638000	-1.524482000	2.008475000
6	-1.416241000	-0.291260000	2.144269000
6	0.720638000	-1.524482000	2.008475000
6	1.416241000	-0.291260000	2.144269000
6	3.546774000	-1.528702000	2.021052000
6	2.857615000	-0.304801000	2.180881000
6	-3.556258000	-3.047899000	0.198004000

6	-2.860728000	-2.570225000	1.349538000
6	-0.705581000	-3.090333000	0.200536000
6	-1.422256000	-2.574660000	1.352845000
6	0.705581000	-3.090333000	0.200536000
6	1.422256000	-2.574660000	1.352845000
6	3.556258000	-3.047899000	0.198004000
6	2.860728000	-2.570225000	1.349538000
6	-3.547630000	-1.831365000	-1.841152000
6	-2.861428000	-2.753107000	-1.013266000
6	-0.720593000	-1.827182000	-1.832031000
6	-1.422355000	-2.758629000	-1.016432000
6	0.720593000	-1.827182000	-1.832031000
6	1.422355000	-2.758629000	-1.016432000
6	3.547630000	-1.831365000	-1.841152000
6	2.861428000	-2.753107000	-1.013266000
6	-3.546520000	0.582355000	-2.004219000
6	-2.858427000	-0.648082000	-2.192567000
6	-0.720020000	0.597307000	-1.934578000
6	-1.416506000	-0.630233000	-2.159726000
6	0.720020000	0.597307000	-1.934578000
6	1.416506000	-0.630233000	-2.159725000
6	3.546520000	0.582355000	-2.004219000
6	2.858427000	-0.648082000	-2.192566000
6	-3.579181000	2.077656000	-0.210972000
6	-2.846405000	1.633827000	-1.373812000
6	-0.798680000	2.552100000	-0.248883000
6	-1.431642000	1.679448000	-1.358461000
6	0.798680000	2.552100000	-0.248883000
6	1.431642000	1.679448000	-1.358461000
6	3.579181000	2.077656000	-0.210973000
6	2.846405000	1.633828000	-1.373813000
6	-3.546110000	0.878865000	1.796167000
6	-2.846752000	1.815317000	1.006193000
6	-0.720360000	0.885264000	1.724309000
6	-1.431622000	1.860373000	0.984164000
6	0.720360000	0.885264000	1.724309000
6	1.431622000	1.860373000	0.984164000
6	3.546110000	0.878865000	1.796167000
6	2.846752000	1.815317000	1.006192000
1	-4.635248000	-1.816338000	-1.826148000
1	-4.643536000	-3.052157000	0.198477000
1	-4.634524000	0.590518000	-2.006216000
1	-4.634382000	-1.516261000	2.004364000
1	-4.655242000	2.203559000	-0.220935000
1	-4.634189000	0.886256000	1.795076000
1	4.635248000	-1.816338000	-1.826148000
1	4.643536000	-3.052157000	0.198477000
1	4.634524000	0.590519000	-2.006217000
1	4.634382000	-1.516261000	2.004364000
1	4.655242000	2.203559000	-0.220935000

1	4.634189000	0.886256000	1.795076000
6	-0.665770000	4.923967000	0.640595000
6	0.665770000	4.923967000	0.640595000
1	-1.256497000	5.511876000	1.334686000
1	1.256497000	5.511875000	1.334686000
6	-1.326293000	4.024151000	-0.361012000
1	-2.409771000	4.047491000	-0.257967000
1	-1.112053000	4.367034000	-1.380832000
6	1.326293000	4.024151000	-0.361012000
1	2.409772000	4.047490000	-0.257967000
1	1.112053000	4.367034000	-1.380832000

Zero-point correction= 0.512975 (Hartree/Particle)
 Thermal correction to Energy= 0.539583
 Thermal correction to Enthalpy= 0.540528
 Thermal correction to Gibbs Free Energy= 0.464401
 Sum of electronic and zero-point Energies= -1991.650438
 Sum of electronic and thermal Energies= -1991.623830
 Sum of electronic and thermal Enthalpies= -1991.622886
Sum of electronic and thermal Free Energies= -1991.699012
Number of imaginary frequencies = 0

(7,0) Adduct

1	-4.629451000	-1.142366000	-2.187405000
6	-2.861695000	0.017417000	-2.600332000
6	-3.541963000	-1.158489000	-2.211717000
6	-1.425194000	0.018050000	-2.520113000
6	-0.720284000	-1.136603000	-2.042734000
6	1.424826000	0.035263000	-2.520146000
6	0.733926000	-1.127800000	-2.042724000
6	2.861240000	0.051951000	-2.600373000
6	3.555674000	-1.115680000	-2.211809000
1	4.642889000	-1.086344000	-2.187471000
1	-4.637526000	1.250429000	-2.586585000
6	-2.890813000	2.356899000	-1.985207000
6	-3.550393000	1.266254000	-2.590408000
6	-1.444020000	2.363141000	-1.962570000
6	-0.724460000	1.254403000	-2.478028000
6	1.415401000	2.380463000	-1.962638000
6	0.709276000	1.263094000	-2.478122000
6	2.862166000	2.391594000	-1.985228000
6	3.534854000	1.308965000	-2.590372000
1	4.622100000	1.306214000	-2.586507000
1	-4.664576000	3.105182000	-1.004835000
6	-2.899936000	3.317993000	0.213504000
6	-3.578048000	3.139870000	-1.015559000
6	-1.448768000	3.333052000	0.226821000
6	-0.733263000	3.138709000	-0.988977000
6	1.408473000	3.350269000	0.226810000
6	0.695361000	3.147358000	-0.989003000

6	2.859713000	3.352687000	0.213488000
6	3.539927000	3.182772000	-1.015587000
1	4.626795000	3.161104000	-1.004837000
1	-4.664633000	2.902462000	1.390336000
6	-2.880568000	2.031795000	2.243518000
6	-3.577854000	2.933314000	1.399165000
6	-1.436033000	2.040335000	2.250418000
6	-0.731476000	2.957447000	1.403372000
6	1.411306000	2.057487000	2.250456000
6	0.695768000	2.966039000	1.403361000
6	2.855834000	2.066284000	2.243492000
6	3.542229000	2.976025000	1.399072000
1	4.629296000	2.958111000	1.390150000
1	-4.636590000	0.822623000	2.597143000
6	-2.848695000	-0.384053000	2.487287000
6	-3.549109000	0.839844000	2.608184000
6	-1.412286000	-0.379835000	2.444169000
6	-0.722146000	0.856424000	2.576243000
6	1.416663000	-0.362823000	2.444317000
6	0.711722000	0.865067000	2.576320000
6	2.853002000	-0.349733000	2.487455000
6	3.538664000	0.882489000	2.608276000
1	4.626272000	0.878334000	2.597070000
1	-4.623429000	-1.467690000	1.887367000
6	-2.857247000	-2.292545000	0.984302000
6	-3.535148000	-1.479810000	1.901960000
6	-1.425067000	-2.336626000	0.980019000
6	-0.717462000	-1.454564000	1.802340000
6	1.453111000	-2.319232000	0.980022000
6	0.734889000	-1.445848000	1.802395000
6	2.884686000	-2.257833000	0.984320000
6	3.552667000	-1.437083000	1.902131000
1	4.640724000	-1.411799000	1.887555000
1	-4.663795000	-2.555463000	-0.226593000
6	-2.872664000	-2.075648000	-1.374844000
6	-3.579907000	-2.561229000	-0.233951000
6	-1.430245000	-2.110628000	-1.348315000
6	-0.782491000	-2.993926000	-0.261395000
6	1.455633000	-2.093129000	-1.348298000
6	0.818578000	-2.984216000	-0.261389000
6	2.897520000	-2.040759000	-1.374823000
6	3.610554000	-2.517678000	-0.233916000
1	4.694285000	-2.498554000	-0.226516000
6	-0.632991000	-5.379360000	0.592062000
6	0.698070000	-5.371246000	0.592097000
1	-1.224540000	-5.973964000	1.279994000
1	1.296779000	-5.958590000	1.280070000
6	-1.295191000	-4.473927000	-0.402089000
1	-2.378658000	-4.498211000	-0.307779000
1	-1.072419000	-4.801521000	-1.425424000

6	1.349236000	-4.457894000	-0.402114000
1	2.432937000	-4.469137000	-0.307912000
1	1.130221000	-4.788144000	-1.425393000

Zero-point correction= 0.584518 (Hartree/Particle)
 Thermal correction to Energy= 0.615764
 Thermal correction to Enthalpy= 0.616708
 Thermal correction to Gibbs Free Energy= 0.531972
 Sum of electronic and zero-point Energies= -2297.736503
 Sum of electronic and thermal Energies= -2297.705258
 Sum of electronic and thermal Enthalpies= -2297.704314
Sum of electronic and thermal Free Energies= -2297.789050
Number of imaginary frequencies = 0

(8,0) Adduct

6	2.997056000	-3.591516000	0.214808000
6	2.612280000	-2.865834000	1.387157000
6	3.499977000	-0.799399000	0.246670000
6	2.664103000	-1.433955000	1.374187000
6	3.499972000	0.799533000	0.246671000
6	2.664067000	1.434073000	1.374193000
6	2.996889000	3.591655000	0.214802000
6	2.612164000	2.865950000	1.387154000
6	1.967384000	-3.549479000	-1.935984000
6	2.750604000	-2.865080000	-0.994215000
6	1.955820000	-0.728358000	-1.832057000
6	2.803510000	-1.433499000	-0.975901000
6	1.955798000	0.728449000	-1.832060000
6	2.803479000	1.433621000	-0.975911000
6	1.967236000	3.549567000	-1.935986000
6	2.750488000	2.865199000	-0.994221000
6	-0.258988000	-3.547539000	-2.928265000
6	0.928279000	-2.855654000	-2.602824000
6	-0.260889000	-0.719453000	-2.882488000
6	0.932285000	-1.416182000	-2.554063000
6	-0.260918000	0.719452000	-2.882485000
6	0.932229000	1.416230000	-2.554057000
6	-0.259135000	3.547537000	-2.928265000
6	0.928160000	2.855703000	-2.602824000
6	-2.613863000	-3.558763000	-2.322504000
6	-1.494442000	-2.868033000	-2.845410000
6	-2.614436000	-0.716957000	-2.312977000
6	-1.489356000	-1.423601000	-2.844439000
6	-2.614466000	0.716858000	-2.312977000
6	-1.489414000	1.423549000	-2.844436000
6	-2.614013000	3.558663000	-2.322510000
6	-1.494561000	2.867980000	-2.845411000
6	-3.772931000	-3.561218000	-0.193214000
6	-3.413763000	-2.875783000	-1.377450000

6	-3.767773000	-0.716926000	-0.192950000
6	-3.419691000	-1.426675000	-1.381701000
6	-3.767804000	0.716781000	-0.192951000
6	-3.419750000	1.426543000	-1.381702000
6	-3.773083000	3.561073000	-0.193219000
6	-3.413885000	2.875652000	-1.377454000
6	-2.876989000	-3.558692000	2.060178000
6	-3.556274000	-2.875788000	1.025279000
6	-2.875555000	-0.716936000	2.050096000
6	-3.562612000	-1.426645000	1.028393000
6	-2.875585000	0.716832000	2.050095000
6	-3.562671000	1.426511000	1.028391000
6	-2.877137000	3.558587000	2.060173000
6	-3.556394000	2.875654000	1.025275000
6	-0.611228000	-3.547976000	2.943836000
6	-1.827519000	-2.868366000	2.713069000
6	-0.607525000	-0.719429000	2.898511000
6	-1.822443000	-1.423711000	2.712696000
6	-0.607553000	0.719420000	2.898507000
6	-1.822500000	1.423652000	2.712690000
6	-0.611373000	3.547966000	2.943828000
6	-1.827636000	2.868306000	2.713062000
6	1.719372000	-3.549900000	2.227682000
6	0.606914000	-2.856224000	2.762529000
6	1.719439000	-0.728457000	2.123932000
6	0.616552000	-1.416531000	2.715948000
6	1.719416000	0.728542000	2.123932000
6	0.616497000	1.416571000	2.715940000
6	1.719227000	3.549982000	2.227678000
6	0.606798000	2.856264000	2.762523000
1	-2.598198000	4.645936000	-2.308369000
1	-0.252200000	4.635319000	-2.921159000
1	-3.742871000	4.648041000	-0.191519000
1	1.954711000	4.637917000	-1.923710000
1	-2.860843000	4.645895000	2.048890000
1	3.040829000	4.674590000	0.217230000
1	-0.603603000	4.635725000	2.936716000
1	1.707920000	4.638290000	2.213940000
1	-2.598003000	-4.646034000	-2.308362000
1	-0.252009000	-4.635321000	-2.921160000
1	-3.742673000	-4.648184000	-0.191512000
1	1.954904000	-4.637829000	-1.923711000
1	-2.860649000	-4.645999000	2.048897000
1	3.041042000	-4.674448000	0.217237000
1	-0.603413000	-4.635735000	2.936727000
1	1.708110000	-4.638209000	2.213950000
6	5.857937000	-0.665843000	-0.686565000
6	5.857954000	0.665922000	-0.686557000
1	6.432816000	-1.257217000	-1.391117000
1	6.432852000	1.257288000	-1.391099000

6	4.979307000	-1.323941000	0.334224000
1	5.000554000	-2.407515000	0.235253000
1	5.340932000	-1.104570000	1.346882000
6	4.979331000	1.324031000	0.334233000
1	5.340956000	1.104640000	1.346887000
1	5.000629000	2.407602000	0.235277000

Zero-point correction= 0.658985 (Hartree/Particle)
 Thermal correction to Energy= 0.693916
 Thermal correction to Enthalpy= 0.694860
 Thermal correction to Gibbs Free Energy= 0.603526
 Sum of electronic and zero-point Energies= -2603.840755
 Sum of electronic and thermal Energies= -2603.805824
 Sum of electronic and thermal Enthalpies= -2603.804880
Sum of electronic and thermal Free Energies= -2603.896214
Number of imaginary frequencies = 0

Optimized Geometries of [5+4] adducts with tube length 9.5 Å

(5,0) Adduct

6	-2.829255000	-2.939482000	-0.958852000
6	-2.006109000	-3.277216000	0.192372000
6	-0.051112000	-2.419185000	-1.060510000
6	-0.666301000	-2.932187000	0.188971000
6	1.293335000	-2.100709000	-1.053155000
6	2.079202000	-2.307287000	0.189434000
6	4.059390000	-1.399869000	-0.943834000
6	3.440150000	-2.029472000	0.192836000
6	-3.368209000	-0.735753000	-1.701975000
6	-2.393493000	-1.816757000	-1.712716000
6	-0.561747000	-0.170816000	-1.874381000
6	-1.002299000	-1.535328000	-1.749607000
6	0.808356000	0.163627000	-1.826596000
6	1.774226000	-0.886418000	-1.707519000
6	3.536190000	0.809151000	-1.777308000
6	3.162447000	-0.559884000	-1.707048000
6	-3.625024000	1.379832000	-0.228480000
6	-2.927465000	0.506025000	-1.298012000
6	-0.968257000	1.413860000	-0.197730000
6	-1.523038000	0.750592000	-1.313232000
6	0.347854000	2.078817000	-0.217804000
6	1.226022000	1.459291000	-1.332143000
6	3.160112000	2.470475000	-0.196656000
6	2.589822000	1.777026000	-1.339187000
6	-3.426715000	-0.448330000	1.581761000
6	-2.966281000	0.712773000	0.993513000
6	-0.633266000	0.135947000	1.740958000
6	-1.564831000	0.944741000	0.998558000
6	0.740735000	0.460997000	1.697953000
6	1.179180000	1.655257000	1.015017000

6	3.467992000	1.099337000	1.656825000
6	2.543864000	1.975764000	1.022390000
6	-2.874683000	-2.748584000	1.232689000
6	-2.463275000	-1.513791000	1.804834000
6	-0.098567000	-2.214615000	1.356900000
6	-1.073658000	-1.229085000	1.844942000
6	1.246011000	-1.898088000	1.348984000
6	1.705709000	-0.589745000	1.806103000
6	4.017333000	-1.216442000	1.231504000
6	3.093736000	-0.262603000	1.805089000
1	-3.864918000	-3.265046000	-1.011843000
1	-3.912698000	-3.064142000	1.298593000
1	-4.424993000	-0.988709000	-1.644672000
1	-4.483288000	-0.704214000	1.533912000
1	-4.702326000	1.206026000	-0.231233000
1	5.136554000	-1.291030000	-1.025511000
1	5.090885000	-1.092081000	1.335567000
1	4.592102000	1.069846000	-1.788801000
1	4.523793000	1.360714000	1.661560000
1	4.178874000	2.837197000	-0.207508000
6	-2.479395000	3.693429000	0.593876000
6	-1.169733000	4.008961000	0.600707000
1	-3.047922000	4.053325000	1.449258000
1	-0.831954000	4.581018000	1.460860000
6	-3.322625000	2.937545000	-0.428324000
1	-4.295099000	3.437519000	-0.459648000
1	-2.887361000	3.060983000	-1.421426000
6	-0.061039000	3.604578000	-0.361522000
1	0.817984000	4.232407000	-0.206948000
1	-0.381356000	3.727908000	-1.399903000

Zero-point correction= 0.440610 (Hartree/Particle)
 Thermal correction to Energy= 0.463154
 Thermal correction to Enthalpy= 0.464098
 Thermal correction to Gibbs Free Energy= 0.395393
 Sum of electronic and zero-point Energies= -1685.539184
 Sum of electronic and thermal Energies= -1685.516640
 Sum of electronic and thermal Enthalpies= -1685.515696
Sum of electronic and thermal Free Energies= -1685.584400
Number of imaginary frequencies = 0

(6,0) Adduct

6	2.844376000	-2.467220000	-2.060492000
6	2.567929000	-1.105557000	-2.223398000
6	0.135262000	-1.630770000	-2.095740000
6	1.189634000	-0.672486000	-2.274265000
6	-1.234906000	-1.188356000	-2.080354000
6	-1.534698000	0.201363000	-2.227562000
6	-3.938846000	-0.305060000	-2.030678000
6	-2.909747000	0.645749000	-2.213659000

6	2.375463000	-3.876319000	-0.197678000
6	1.866848000	-3.236333000	-1.355413000
6	-0.326400000	-3.030263000	-0.198929000
6	0.497442000	-2.796505000	-1.360786000
6	-1.679224000	-2.602182000	-0.198655000
6	-2.215558000	-1.939336000	-1.361009000
6	-4.389219000	-1.738835000	-0.198531000
6	-3.587017000	-1.496753000	-1.350448000
6	2.746820000	-2.775425000	1.880913000
6	1.806836000	-3.423827000	1.017750000
6	0.037139000	-1.941739000	1.911664000
6	0.438170000	-2.983185000	1.024578000
6	-1.332995000	-1.500128000	1.899549000
6	-2.275434000	-2.130504000	1.026247000
6	-4.036326000	-0.614446000	1.853781000
6	-3.646427000	-1.689059000	1.017848000
6	3.495034000	-0.471801000	1.931285000
6	2.460401000	-1.452139000	2.227033000
6	0.759748000	0.353400000	2.095598000
6	1.078480000	-1.023091000	2.280638000
6	-0.604246000	0.801372000	2.040968000
6	-1.645926000	-0.147613000	2.237054000
6	-3.282245000	1.681266000	2.010515000
6	-3.020495000	0.297729000	2.220663000
6	3.887435000	1.465038000	0.237938000
6	3.118686000	0.699368000	1.332038000
6	1.222056000	1.703683000	0.207572000
6	1.739623000	1.086292000	1.359692000
6	-0.025047000	2.494833000	0.228885000
6	-0.936156000	2.026549000	1.381594000
6	-2.814132000	3.105772000	0.199852000
6	-2.277308000	2.445865000	1.367042000
6	3.581841000	-0.177087000	-1.747669000
6	3.173109000	0.889087000	-0.990789000
6	0.856447000	0.659331000	-1.888254000
6	1.793627000	1.261065000	-1.000596000
6	-0.506652000	1.105036000	-1.846185000
6	-0.866326000	2.230448000	-1.038889000
6	-3.180706000	1.988196000	-1.822125000
6	-2.206834000	2.647720000	-1.028600000
1	3.788856000	-3.081513000	1.819715000
1	3.421558000	-4.173951000	-0.194892000
1	4.527478000	-0.811604000	1.871438000
1	3.883777000	-2.781810000	-1.997220000
1	4.942236000	1.183852000	0.240450000
1	4.615533000	-0.515776000	-1.704652000
1	-5.067085000	-0.268434000	1.824462000
1	-5.425982000	-1.411500000	-0.198417000
1	-4.311027000	2.034984000	2.006314000
1	-4.970568000	0.037726000	-1.997321000

1	-3.794410000	3.566842000	0.210863000
1	-4.208235000	2.345408000	-1.818049000
6	2.961010000	3.877188000	-0.582374000
6	1.680686000	4.295936000	-0.574868000
1	3.549924000	4.196777000	-1.440096000
1	1.378850000	4.898101000	-1.427876000
6	3.747178000	3.050095000	0.428839000
1	4.765175000	3.450149000	0.437382000
1	3.343390000	3.221046000	1.428549000
6	0.562291000	3.970374000	0.398492000
1	-0.257597000	4.684736000	0.286219000
1	0.913908000	4.024547000	1.432625000

Zero-point correction= 0.515248 (Hartree/Particle)
 Thermal correction to Energy= 0.541633
 Thermal correction to Enthalpy= 0.542577
 Thermal correction to Gibbs Free Energy= 0.466967
 Sum of electronic and zero-point Energies= -1991.676675
 Sum of electronic and thermal Energies= -1991.650291
 Sum of electronic and thermal Enthalpies= -1991.649347
Sum of electronic and thermal Free Energies= -1991.724956
Number of imaginary frequencies = 0

(7,0) Adduct

1	4.342908000	1.883393000	2.023791000
6	2.209858000	1.711138000	2.538479000
6	3.492108000	1.204684000	2.046041000
6	1.071661000	0.811818000	2.598369000
6	1.228393000	-0.551843000	2.240334000
6	-1.155226000	-0.969794000	2.593607000
6	0.126006000	-1.451529000	2.196556000
6	-2.289309000	-1.860985000	2.563992000
6	-2.070182000	-3.204612000	2.149329000
1	-2.909674000	-3.896842000	2.138173000
1	2.843422000	3.749945000	2.449280000
6	0.722524000	3.554680000	2.018031000
6	1.989698000	3.078431000	2.510160000
6	-0.402532000	2.654742000	2.022307000
6	-0.260359000	1.342398000	2.568012000
6	-2.625933000	0.866371000	2.009573000
6	-1.372032000	0.439962000	2.554627000
6	-3.764836000	-0.023942000	1.986488000
6	-3.596543000	-1.336641000	2.497473000
1	-4.435583000	-2.027105000	2.451698000
1	1.636221000	5.244858000	1.060584000
6	0.075096000	4.358713000	-0.157881000
6	0.770428000	4.586855000	1.074541000
6	-1.038422000	3.456473000	-0.163494000
6	-1.443434000	2.818733000	1.056600000
6	-3.250536000	1.653454000	-0.172117000

6	-2.551545000	1.921244000	1.052846000
6	-4.389420000	0.769060000	-0.188688000
6	-4.802149000	0.192110000	1.046339000
1	-5.633379000	-0.508434000	1.031040000
1	1.729561000	5.141043000	-1.296363000
6	0.885856000	3.368614000	-2.200737000
6	0.862276000	4.485306000	-1.322101000
6	-0.237395000	2.476334000	-2.219402000
6	-1.345609000	2.714623000	-1.346032000
6	-2.466610000	0.679875000	-2.214769000
6	-2.457736000	1.817110000	-1.347362000
6	-3.608941000	-0.205196000	-2.230318000
6	-4.719082000	0.105213000	-1.395186000
1	-5.550826000	-0.594613000	-1.380545000
1	3.025492000	3.538859000	-2.466962000
6	2.396055000	1.484761000	-2.447095000
6	2.173431000	2.866044000	-2.536171000
6	1.266331000	0.594129000	-2.502850000
6	-0.054727000	1.114023000	-2.618320000
6	-0.979987000	-1.192155000	-2.484280000
6	-1.175723000	0.212761000	-2.611245000
6	-2.113964000	-2.080342000	-2.507312000
6	-3.417194000	-1.537714000	-2.665220000
1	-4.264637000	-2.218237000	-2.638380000
1	4.482377000	1.699790000	-1.805715000
6	3.584239000	-0.069002000	-1.011000000
6	3.627836000	1.025997000	-1.829603000
6	2.417191000	-0.890398000	-1.012747000
6	1.381207000	-0.727223000	-1.949146000
6	0.237525000	-2.713115000	-1.008198000
6	0.254446000	-1.616770000	-1.892258000
6	-0.902333000	-3.567488000	-1.000655000
6	-1.955218000	-3.362909000	-1.922792000
1	-2.815612000	-4.027714000	-1.884570000
1	5.350398000	0.279888000	0.204511000
6	3.499177000	0.053491000	1.323593000
6	4.464991000	-0.358704000	0.205104000
6	2.334760000	-0.797928000	1.348880000
6	2.039205000	-1.520926000	0.210296000
6	0.207344000	-2.660761000	1.432038000
6	1.167683000	-2.718522000	0.224525000
6	-0.907823000	-3.510150000	1.404608000
6	-1.257441000	-4.243926000	0.207939000
1	-2.057687000	-4.974144000	0.221049000
6	4.429293000	-2.900898000	-0.692949000
6	3.377690000	-3.743504000	-0.700029000
1	5.062765000	-2.940013000	-1.577302000
1	3.282842000	-4.362871000	-1.588590000
6	4.900032000	-1.896481000	0.350863000
1	5.993593000	-1.910682000	0.338014000

1	4.598346000	-2.231141000	1.344952000
6	2.245354000	-3.893787000	0.300565000
1	1.741525000	-4.852471000	0.156645000
1	2.625211000	-3.864930000	1.325730000

Zero-point correction= 0.586343 (Hartree/Particle)
 Thermal correction to Energy= 0.617330
 Thermal correction to Enthalpy= 0.618274
 Thermal correction to Gibbs Free Energy= 0.534113
 Sum of electronic and zero-point Energies= -2297.757113
 Sum of electronic and thermal Energies= -2297.726126
 Sum of electronic and thermal Enthalpies= -2297.725182
Sum of electronic and thermal Free Energies= -2297.809343
Number of imaginary frequencies = 0

(8,0) Adduct

6	4.425730000	1.890302000	-0.233876000
6	3.405946000	1.723112000	-1.365102000
6	2.947880000	-0.364560000	-0.207480000
6	2.853807000	0.397021000	-1.378385000
6	2.833600000	-1.841259000	-0.220391000
6	1.950985000	-2.296235000	-1.389037000
6	1.580454000	-4.427458000	-0.189099000
6	1.444864000	-3.626344000	-1.369872000
6	3.068562000	2.606998000	1.866678000
6	3.537626000	1.675690000	0.988404000
6	2.057912000	-0.055310000	1.986874000
6	2.969432000	0.359967000	0.993270000
6	1.573289000	-1.417366000	1.956318000
6	2.104061000	-2.342092000	1.036247000
6	0.636375000	-4.065541000	1.983190000
6	1.596265000	-3.669798000	1.029108000
6	0.972342000	3.373553000	2.905046000
6	1.841886000	2.333521000	2.599391000
6	-0.013749000	0.711475000	2.990205000
6	1.353076000	0.969580000	2.659144000
6	-0.497800000	-0.647983000	2.992741000
6	0.385542000	-1.721667000	2.677412000
6	-1.461376000	-3.325346000	2.988176000
6	-0.105921000	-3.076367000	2.678212000
6	-1.251105000	4.157174000	2.306426000
6	-0.437962000	3.148094000	2.843434000
6	-2.214610000	1.487629000	2.323122000
6	-0.927506000	1.787282000	2.871407000
6	-2.693481000	0.135933000	2.327785000
6	-1.892701000	-0.900311000	2.904046000
6	-3.660231000	-2.537986000	2.343274000
6	-2.385038000	-2.261010000	2.894866000
6	-2.343693000	4.534560000	0.178565000
6	-2.244343000	3.778568000	1.367029000

6	-3.278129000	1.856671000	0.183877000
6	-2.726151000	2.416659000	1.374335000
6	-3.747962000	0.505042000	0.185497000
6	-3.673895000	-0.270645000	1.380472000
6	-4.721191000	-2.163701000	0.192366000
6	-4.160825000	-1.634700000	1.378787000
6	-1.491429000	4.233751000	-2.068808000
6	-2.375833000	3.820771000	-1.038364000
6	-2.453677000	1.564484000	-2.069969000
6	-2.856341000	2.458551000	-1.039446000
6	-2.934545000	0.213545000	-2.071328000
6	-3.806784000	-0.227403000	-1.037307000
6	-3.905257000	-2.458155000	-2.074570000
6	-4.293411000	-1.591161000	-1.029692000
6	0.651838000	3.476645000	-2.933910000
6	-0.744261000	3.245987000	-2.725426000
6	-0.341833000	0.816730000	-3.007570000
6	-1.234521000	1.885485000	-2.746357000
6	-0.828467000	-0.542128000	-3.006838000
6	-2.206943000	-0.798815000	-2.771753000
6	-1.795344000	-3.218665000	-2.987122000
6	-2.699414000	-2.158865000	-2.756365000
6	2.841802000	2.685376000	-2.146698000
6	1.547296000	2.429450000	-2.762797000
6	1.832591000	0.016506000	-2.280322000
6	1.056153000	1.064720000	-2.825771000
6	1.340902000	-1.344026000	-2.228479000
6	0.079407000	-1.625237000	-2.826162000
6	0.391118000	-3.990857000	-2.231344000
6	-0.413385000	-2.979528000	-2.816627000
1	-4.011568000	-3.566994000	2.330845000
1	-1.829173000	-4.348667000	2.963591000
1	-5.063523000	-3.195757000	0.192741000
1	0.261504000	-5.087137000	1.962896000
1	-4.254661000	-3.487778000	-2.059601000
1	1.257693000	-5.461972000	-0.188276000
1	-2.161429000	-4.242497000	-2.957471000
1	0.015354000	-5.011968000	-2.203527000
1	-0.863108000	5.172424000	2.265855000
1	1.330901000	4.398481000	2.837118000
1	-1.947775000	5.547419000	0.174864000
1	3.454348000	3.624854000	1.855440000
1	-1.100731000	5.248231000	-2.036663000
1	4.844306000	2.898431000	-0.237678000
1	1.016718000	4.499121000	-2.863557000
1	3.215772000	3.707607000	-2.127268000
6	5.742540000	-0.305646000	0.642174000
6	5.284490000	-1.572364000	0.631970000
1	6.324348000	-0.027505000	1.518889000
1	5.542969000	-2.170589000	1.502041000

6	5.606966000	0.812834000	-0.383957000
1	6.544272000	1.375974000	-0.366160000
1	5.527141000	0.381966000	-1.383992000
6	4.371721000	-2.263962000	-0.362364000
1	4.647751000	-2.011578000	-1.390714000
1	4.444805000	-3.349121000	-0.252936000
Zero-point correction=			0.661358 (Hartree/Particle)
Thermal correction to Energy=			0.696039
Thermal correction to Enthalpy=			0.696984
Thermal correction to Gibbs Free Energy=			0.606230
Sum of electronic and zero-point Energies=			-2603.876333
Sum of electronic and thermal Energies=			-2603.841652
Sum of electronic and thermal Enthalpies=			-2603.840708
Sum of electronic and thermal Free Energies=			-2603.931462
Number of imaginary frequencies = 0			

Optimized Geometries of pristine tubes with different length

(5,0)CNT with 11.34Å

6	1.697451000	4.599477000	1.086436000
6	2.281416000	3.847771000	0.001181000
6	1.719957000	1.765871000	1.203596000
6	2.238328000	2.475789000	-0.001083000
6	1.716729000	0.385611000	1.207333000
6	2.172327000	-0.337336000	-0.002505000
6	1.714376000	-2.455884000	1.167278000
6	2.196479000	-1.718966000	-0.002328000
6	1.758448000	-3.868348000	1.192328000
6	2.154020000	-4.561632000	0.001019000
6	-0.644117000	4.593205000	1.743643000
6	0.590454000	3.923001000	1.742327000
6	-0.638238000	1.760604000	1.834093000
6	0.599235000	2.489919000	1.768338000
6	-0.628972000	0.348743000	1.839394000
6	0.621505000	-0.349127000	1.833208000
6	-0.604546000	-2.491015000	1.774328000
6	0.632552000	-1.758576000	1.828937000
6	-0.591362000	-3.926110000	1.748135000
6	0.648653000	-4.592096000	1.744003000
6	-2.150276000	4.567806000	0.000696000
6	-1.758211000	3.874948000	1.192721000
6	-2.203210000	1.722385000	-0.000750000
6	-1.721408000	2.459876000	1.170451000
6	-2.179353000	0.337660000	-0.001017000
6	-1.726553000	-0.385657000	1.211259000
6	-2.241943000	-2.478635000	0.000173000
6	-1.728103000	-1.768728000	1.206647000
6	-2.283429000	-3.854536000	0.001250000
6	-1.693136000	-4.607031000	1.082686000
6	-0.645921000	4.597190000	-1.740875000

6	-1.757196000	3.875775000	-1.190752000
6	-0.638355000	1.761181000	-1.836333000
6	-1.718980000	2.460470000	-1.169989000
6	-0.628658000	0.350170000	-1.842118000
6	-1.722942000	-0.385945000	-1.211155000
6	-0.603203000	-2.493508000	-1.773162000
6	-1.724454000	-1.769432000	-1.205350000
6	-0.590036000	-3.927765000	-1.743897000
6	-1.691144000	-4.608006000	-1.078062000
6	1.698532000	4.603198000	-1.082357000
6	0.592301000	3.927695000	-1.744963000
6	1.723733000	1.768849000	-1.207658000
6	0.601548000	2.493154000	-1.774036000
6	1.720903000	0.385168000	-1.213422000
6	0.624812000	-0.349064000	-1.843735000
6	1.719498000	-2.456203000	-1.173118000
6	0.636000000	-1.759873000	-1.838434000
6	1.760782000	-3.871761000	-1.192332000
6	0.648904000	-4.595081000	-1.740193000
1	-0.653878000	5.680446000	1.732737000
1	1.866129000	5.661823000	1.214455000
1	-2.230817000	5.651608000	0.001519000
1	1.866433000	5.669238000	-1.202980000
1	-0.660730000	5.684199000	-1.731099000
1	-1.854596000	-5.673020000	1.208533000
1	0.666727000	-5.678833000	1.731838000
1	-1.852021000	-5.674444000	-1.202069000
1	2.236179000	-5.645097000	0.003060000
1	0.665872000	-5.681998000	-1.727834000

Zero-point correction= 0.408669 (Hartree/Particle)
 Thermal correction to Energy= 0.431854
 Thermal correction to Enthalpy= 0.432798
 Thermal correction to Gibbs Free Energy= 0.362740
 Sum of electronic and zero-point Energies= -1910.456690
 Sum of electronic and thermal Energies= -1910.433506
 Sum of electronic and thermal Enthalpies= -1910.432561
Sum of electronic and thermal Free Energies= -1910.502619
Number of imaginary frequencies = 0

(5,0)CNT with 13.49Å

6	1.550785000	5.664726000	1.040849000
6	2.108610000	4.954001000	-0.066655000
6	1.618313000	2.829724000	1.130463000
6	2.067807000	3.533319000	-0.050570000
6	1.626184000	1.419349000	1.145174000
6	2.092654000	0.682723000	-0.024029000
6	1.644423000	-1.422163000	1.175230000
6	2.097188000	-0.708233000	-0.017349000
6	1.665023000	-2.818588000	1.197945000

6	2.085878000	-3.547740000	-0.006868000
6	1.618536000	-5.660667000	1.137607000
6	2.115712000	-4.955024000	-0.003121000
6	-0.728888000	5.656424000	1.890156000
6	0.557540000	4.991243000	1.766184000
6	-0.663556000	2.829628000	1.967107000
6	0.566847000	3.553188000	1.792502000
6	-0.651005000	1.436445000	1.955899000
6	0.608818000	0.713211000	1.876108000
6	-0.643862000	-1.405447000	1.926470000
6	0.612172000	-0.693813000	1.891372000
6	-0.645517000	-2.813203000	1.942258000
6	0.605865000	-3.534227000	1.870700000
6	-0.624019000	-5.660182000	1.854310000
6	0.616528000	-4.966032000	1.896054000
6	-2.016676000	5.663720000	0.115917000
6	-1.836358000	4.909353000	1.336362000
6	-2.088081000	2.832669000	0.021404000
6	-1.801885000	3.533165000	1.306167000
6	-2.080261000	1.442761000	0.009776000
6	-1.720723000	0.713373000	1.242626000
6	-2.062624000	-1.406101000	0.012546000
6	-1.711262000	-0.677399000	1.235149000
6	-2.089693000	-2.808985000	0.012207000
6	-1.663069000	-3.534039000	1.198131000
6	-2.029528000	-5.658214000	0.016978000
6	-1.691718000	-4.957476000	1.217866000
6	-0.494634000	5.672083000	-1.783941000
6	-1.505708000	4.998658000	-1.073153000
6	-0.571486000	2.835891000	-1.883804000
6	-1.533835000	3.561787000	-1.096738000
6	-0.586667000	1.422447000	-1.893106000
6	-1.614935000	0.716498000	-1.169081000
6	-0.609786000	-1.420997000	-1.902594000
6	-1.633914000	-0.689790000	-1.179026000
6	-0.622683000	-2.826585000	-1.914509000
6	-1.630383000	-3.536176000	-1.156790000
6	-0.602109000	-5.665351000	-1.824470000
6	-1.664704000	-4.961596000	-1.179620000
6	1.803345000	5.628270000	-1.295712000
6	0.727601000	4.957026000	-1.979669000
6	1.751033000	2.801360000	-1.265084000
6	0.694499000	3.535829000	-1.948572000
6	1.717476000	1.401150000	-1.241313000
6	0.666491000	0.685367000	-1.965467000
6	1.706442000	-1.438899000	-1.232308000
6	0.658679000	-0.711338000	-1.961960000
6	1.715511000	-2.827820000	-1.233140000
6	0.635494000	-3.555369000	-1.894259000
6	1.661662000	-5.674862000	-1.167415000

6	0.639910000	-4.976180000	-1.909869000
1	-0.788885000	6.723268000	2.085841000
1	1.532278000	6.748736000	1.008868000
1	-2.217916000	6.730738000	0.119058000
1	1.851636000	6.714067000	-1.325291000
1	-0.467822000	6.758439000	-1.754383000
1	-0.638605000	-6.746168000	1.896499000
1	-2.104737000	-6.742273000	0.018110000
1	1.691304000	-6.743439000	1.191655000
1	-0.621442000	-6.751347000	-1.866047000
1	1.762022000	-6.753819000	-1.235638000

Zero-point correction= 0.469138 (Hartree/Particle)
 Thermal correction to Energy= 0.496383
 Thermal correction to Enthalpy= 0.497327
 Thermal correction to Gibbs Free Energy= 0.419369
 Sum of electronic and zero-point Energies= -2291.393074
 Sum of electronic and thermal Energies= -2291.365829
 Sum of electronic and thermal Enthalpies= -2291.364884
Sum of electronic and thermal Free Energies= -2291.442842
Number of imaginary frequencies = 0

(5,0)CNT with 15.63Å

6	1.604636000	6.725922000	1.167223000
6	2.049551000	6.025933000	0.001718000
6	1.666653000	3.885193000	1.211444000
6	2.013438000	4.607936000	-0.000631000
6	1.645092000	2.485567000	1.195568000
6	2.048340000	1.764166000	-0.002864000
6	1.650441000	-0.359549000	1.198748000
6	2.039220000	0.362691000	-0.002822000
6	1.663725000	-1.760392000	1.207931000
6	2.043120000	-2.483256000	-0.000434000
6	1.636715000	-4.607476000	1.187477000
6	2.067467000	-3.885945000	0.000542000
6	1.666210000	-6.027904000	1.208292000
6	1.986396000	-6.729880000	0.002167000
6	-0.610663000	6.730222000	1.886193000
6	0.633164000	6.025486000	1.950077000
6	-0.640211000	3.888458000	1.962333000
6	0.620333000	4.607493000	1.915992000
6	-0.634279000	2.484966000	1.938921000
6	0.629670000	1.763694000	1.949306000
6	-0.635229000	-0.359847000	1.945495000
6	0.627303000	0.362178000	1.940270000
6	-0.636241000	-1.764152000	1.956052000
6	0.631590000	-2.483871000	1.942148000
6	-0.621159000	-4.609977000	1.920407000
6	0.640335000	-3.886621000	1.964370000
6	-0.629767000	-6.030440000	1.953524000

6	0.617844000	-6.730170000	1.885593000
6	-1.983821000	6.735840000	0.000659000
6	-1.661317000	6.032267000	1.206451000
6	-2.068173000	3.890128000	-0.001041000
6	-1.635648000	4.611481000	1.184998000
6	-2.044335000	2.487237000	-0.001805000
6	-1.668724000	1.764319000	1.206908000
6	-2.048927000	-0.362739000	-0.001646000
6	-1.660146000	0.360729000	1.201072000
6	-2.057073000	-1.766395000	-0.000839000
6	-1.651170000	-2.487772000	1.198978000
6	-2.017286000	-4.612805000	0.000290000
6	-1.668768000	-3.889882000	1.213520000
6	-2.049801000	-6.033125000	0.001171000
6	-1.596842000	-6.733562000	1.165132000
6	-0.614227000	6.736103000	-1.883715000
6	-1.662669000	6.033912000	-1.205671000
6	-0.640936000	3.890821000	-1.964589000
6	-1.635462000	4.613170000	-1.186469000
6	-0.634058000	2.487853000	-1.942399000
6	-1.665914000	1.764843000	-1.209474000
6	-0.634613000	-0.362183000	-1.948053000
6	-1.657112000	0.360478000	-1.203519000
6	-0.635971000	-1.765888000	-1.956487000
6	-1.651306000	-2.488952000	-1.200060000
6	-0.621871000	-4.612252000	-1.919827000
6	-1.669849000	-3.891004000	-1.213830000
6	-0.630524000	-6.032549000	-1.951549000
6	-1.597957000	-6.735004000	-1.162567000
6	1.603455000	6.731384000	-1.160419000
6	0.632838000	6.033287000	-1.950023000
6	1.667900000	3.889198000	-1.213651000
6	0.620878000	4.612327000	-1.919894000
6	1.647567000	2.485867000	-1.201108000
6	0.632056000	1.765320000	-1.959240000
6	1.654115000	-0.359033000	-1.205069000
6	0.629513000	0.361551000	-1.949906000
6	1.664313000	-1.763138000	-1.209878000
6	0.631065000	-2.486813000	-1.941742000
6	1.635904000	-4.609101000	-1.185484000
6	0.639803000	-3.889057000	-1.963280000
6	1.665478000	-6.029414000	-1.204721000
6	0.617084000	-6.732332000	-1.881580000
1	-0.631358000	7.813564000	1.970776000
1	1.680784000	7.806085000	1.222565000
1	-2.070812000	7.818892000	0.001990000
1	1.676542000	7.814823000	-1.205222000
1	-0.640049000	7.819185000	-1.966406000
1	0.645098000	-7.813499000	1.966028000
1	-1.662711000	-7.817098000	1.214522000

1	2.071595000	-7.813190000	0.002875000
1	-1.664533000	-7.818529000	-1.211156000
1	0.644275000	-7.815772000	-1.960651000

Zero-point correction= 0.529549 (Hartree/Particle)
 Thermal correction to Energy= 0.560726
 Thermal correction to Enthalpy= 0.561670
 Thermal correction to Gibbs Free Energy= 0.476484
 Sum of electronic and zero-point Energies= -2672.338098
 Sum of electronic and thermal Energies= -2672.306921
 Sum of electronic and thermal Enthalpies= -2672.305977
Sum of electronic and thermal Free Energies= -2672.391163
Number of imaginary frequencies = 0

Optimized Geometries of TSs with different length

(5,0)CNT_{TS} of 11.34Å

6	-4.555836000	1.493410000	-0.221256000
6	-3.879302000	0.780984000	-1.320491000
6	-1.902003000	1.702426000	-0.229791000
6	-2.465906000	0.892520000	-1.296187000
6	-0.427281000	2.037130000	-0.236874000
6	0.349123000	1.240036000	-1.333589000
6	2.409356000	2.000832000	-0.207020000
6	1.731171000	1.372128000	-1.353428000
6	3.799725000	2.168949000	-0.209752000
6	4.574840000	1.624778000	-1.289721000
6	-4.477915000	-0.081667000	1.668770000
6	-3.899469000	1.002403000	1.000108000
6	-1.663167000	0.177194000	1.677167000
6	-2.489304000	1.118766000	0.973683000
6	-0.262500000	0.335023000	1.668533000
6	0.327260000	1.456563000	1.001729000
6	2.533894000	0.643051000	1.731953000
6	1.708626000	1.594200000	1.024475000
6	3.959395000	0.803704000	1.761212000
6	4.553058000	1.834987000	0.966121000
6	-4.235735000	-2.403888000	1.273967000
6	-3.659229000	-1.249190000	1.867230000
6	-1.394098000	-2.217948000	1.366946000
6	-2.239703000	-1.122270000	1.847978000
6	-0.018775000	-2.062445000	1.356544000
6	0.573884000	-0.823894000	1.868492000
6	2.808143000	-1.716723000	1.325293000
6	1.963679000	-0.671390000	1.895756000
6	4.213121000	-1.572371000	1.349395000
6	4.779098000	-0.360087000	1.843751000
6	-4.215110000	-2.615928000	-0.968354000
6	-3.459637000	-2.983087000	0.204501000

6	-1.371402000	-2.446692000	-1.043956000
6	-2.063158000	-2.810829000	0.200883000
6	0.004128000	-2.286864000	-1.035962000
6	0.774205000	-2.549750000	0.202919000
6	2.831090000	-1.934967000	-1.013718000
6	2.145314000	-2.396290000	0.202361000
6	4.236370000	-1.794032000	-1.035825000
6	4.976447000	-1.965033000	0.190384000
6	-4.447615000	-0.408042000	-1.789897000
6	-3.626305000	-1.592060000	-1.757633000
6	-1.628623000	-0.155248000	-1.806721000
6	-2.206047000	-1.463950000	-1.738848000
6	-0.228978000	0.009676000	-1.795881000
6	0.609379000	-1.164100000	-1.758573000
6	2.568523000	0.307516000	-1.857206000
6	1.999753000	-1.015468000	-1.783859000
6	3.994212000	0.462242000	-1.888544000
6	4.813561000	-0.694655000	-1.737086000
1	-5.560230000	-0.194749000	1.666523000
1	-5.634893000	1.617817000	-0.243975000
1	-5.310077000	-2.563138000	1.318823000
1	-5.529850000	-0.521930000	-1.787228000
1	-5.288727000	-2.782502000	-1.001543000
6	-2.436676000	4.320952000	0.582766000
6	-1.084739000	4.343994000	0.627192000
1	-2.992017000	4.789167000	1.391749000
1	-0.579400000	4.846348000	1.444629000
6	-3.199088000	3.658823000	-0.453685000
1	-4.258820000	3.873706000	-0.449502000
1	-2.790231000	3.634374000	-1.456950000
6	-0.261282000	3.606595000	-0.377253000
1	0.793212000	3.862460000	-0.288868000
1	-0.567116000	3.846921000	-1.400283000
1	5.624101000	2.011443000	1.007499000
1	5.646836000	1.792048000	-1.342510000
1	5.859491000	-0.249669000	1.893351000
1	5.894844000	-0.592695000	-1.784966000
1	6.062078000	-1.949692000	0.199258000

Zero-point correction=	0.498672 (Hartree/Particle)
Thermal correction to Energy=	0.525167
Thermal correction to Enthalpy=	0.526111
Thermal correction to Gibbs Free Energy=	0.450210
Sum of electronic and zero-point Energies=	-2066.412294
Sum of electronic and thermal Energies=	-2066.385799
Sum of electronic and thermal Enthalpies=	-2066.384855
Sum of electronic and thermal Free Energies=	-2066.460756
Number of imaginary frequencies = 1 (-443.6453)	

(5,0)CNT_{TS} of 13.49Å

6	-5.534883000	1.559099000	-0.220743000
6	-4.867783000	0.839150000	-1.319999000
6	-2.864436000	1.713833000	-0.229237000
6	-3.449670000	0.921115000	-1.296705000
6	-1.383024000	2.011034000	-0.235781000
6	-0.622846000	1.204556000	-1.339579000
6	1.452204000	1.926693000	-0.204859000
6	0.759540000	1.304007000	-1.353969000
6	2.827539000	2.049095000	-0.205463000
6	3.603619000	1.518890000	-1.325478000
6	5.685125000	2.186056000	-0.194862000
6	5.019209000	1.656208000	-1.349706000
6	-5.484299000	-0.005685000	1.677066000
6	-4.883439000	1.060764000	0.999736000
6	-2.662314000	0.190404000	1.683120000
6	-3.468809000	1.147569000	0.974374000
6	-1.254887000	0.318206000	1.676343000
6	-0.641165000	1.424907000	1.010683000
6	1.543207000	0.571576000	1.771291000
6	0.740336000	1.528264000	1.030028000
6	2.948918000	0.699534000	1.792747000
6	3.584973000	1.737207000	1.005490000
6	5.779592000	0.927539000	1.747823000
6	5.000219000	1.879684000	1.028100000
6	-5.289514000	-2.329651000	1.276119000
6	-4.691595000	-1.191372000	1.868581000
6	-2.444528000	-2.202966000	1.361249000
6	-3.263632000	-1.093760000	1.846010000
6	-1.060971000	-2.071755000	1.345899000
6	-0.443253000	-0.858394000	1.882786000
6	1.774306000	-1.811713000	1.353455000
6	0.947201000	-0.738360000	1.911134000
6	3.155456000	-1.690695000	1.363088000
6	3.773407000	-0.482482000	1.884246000
6	5.989974000	-1.380726000	1.285075000
6	5.198071000	-0.359271000	1.912986000
6	-5.273198000	-2.542796000	-0.974563000
6	-4.530086000	-2.919360000	0.202152000
6	-2.426063000	-2.431602000	-1.041133000
6	-3.125538000	-2.775389000	0.198783000
6	-1.042514000	-2.295396000	-1.028421000
6	-0.276430000	-2.580328000	0.202279000
6	1.793703000	-2.036121000	-1.038285000
6	1.097228000	-2.445565000	0.200986000
6	3.174918000	-1.916603000	-1.047628000
6	3.927822000	-2.143272000	0.195618000
6	6.008314000	-1.593140000	-0.983719000
6	5.330095000	-2.043508000	0.197548000
6	-5.460281000	-0.333669000	-1.799763000
6	-4.665370000	-1.534481000	-1.760642000

6	-2.634128000	-0.143597000	-1.812699000
6	-3.236519000	-1.435414000	-1.738491000
6	-1.227095000	-0.009407000	-1.802781000
6	-0.413624000	-1.202101000	-1.772645000
6	1.572667000	0.228041000	-1.893564000
6	0.977306000	-1.086188000	-1.797967000
6	2.978702000	0.351926000	-1.915412000
6	3.802845000	-0.825466000	-1.774870000
6	5.808796000	0.589074000	-1.868455000
6	5.227957000	-0.706908000	-1.802144000
1	-6.568670000	-0.096501000	1.672863000
1	-6.613498000	1.687125000	-0.241744000
1	-6.369156000	-2.453916000	1.308675000
1	-6.544621000	-0.424996000	-1.795533000
1	-6.352483000	-2.671787000	-0.997824000
6	-3.330878000	4.353836000	0.585595000
6	-1.977332000	4.336963000	0.626702000
1	-3.871061000	4.832462000	1.398747000
1	-1.455093000	4.820047000	1.445106000
6	-4.110647000	3.721849000	-0.451256000
1	-5.167333000	3.947282000	-0.441667000
1	-3.702805000	3.675962000	-1.453620000
6	-1.180595000	3.578545000	-0.380726000
1	-0.119028000	3.805146000	-0.299211000
1	-1.485660000	3.824130000	-1.402618000
1	6.758703000	2.350570000	-0.201975000
1	6.861008000	1.034365000	1.781738000
1	6.890857000	0.689035000	-1.901978000
1	7.074052000	-1.354154000	1.347949000
1	7.093366000	-1.575662000	-1.032191000

Zero-point correction= 0.560333 (Hartree/Particle)
 Thermal correction to Energy= 0.590691
 Thermal correction to Enthalpy= 0.591635
 Thermal correction to Gibbs Free Energy= 0.508930
 Sum of electronic and zero-point Energies= -2447.346235
 Sum of electronic and thermal Energies= -2447.315877
 Sum of electronic and thermal Enthalpies= -2447.314933
Sum of electronic and thermal Free Energies= -2447.397639
Number of imaginary frequencies = 1 (-416.1850)

(5,0)CNT_{TS} of 15.63Å

6	-6.534295000	1.616324000	-0.221547000
6	-5.873591000	0.891983000	-1.320389000
6	-3.850128000	1.729821000	-0.230162000
6	-4.452526000	0.951396000	-1.298458000
6	-2.364877000	2.002490000	-0.236962000
6	-1.617549000	1.185848000	-1.342771000
6	0.469823000	1.879760000	-0.206089000
6	-0.232559000	1.259441000	-1.351496000

6	1.844646000	1.964229000	-0.205174000
6	2.610179000	1.441245000	-1.347511000
6	4.697920000	2.088657000	-0.198087000
6	4.006089000	1.544413000	-1.360048000
6	6.112292000	2.212658000	-0.200851000
6	6.854974000	1.679134000	-1.300747000
6	-6.503715000	0.062187000	1.683219000
6	-5.885819000	1.115034000	0.998164000
6	-3.677198000	0.210129000	1.685938000
6	-4.468389000	1.179405000	0.974037000
6	-2.264347000	0.314856000	1.677289000
6	-1.632768000	1.409342000	1.012269000
6	0.537441000	0.525256000	1.784414000
6	-0.248692000	1.485640000	1.027124000
6	1.941012000	0.630567000	1.807882000
6	2.594642000	1.666899000	1.025025000
6	4.777188000	0.820569000	1.792823000
6	3.990204000	1.772924000	1.037152000
6	6.205109000	0.927871000	1.824048000
6	6.839886000	1.896824000	0.989082000
6	-6.344856000	-2.263630000	1.278994000
6	-5.731276000	-1.136180000	1.870145000
6	-3.499515000	-2.181946000	1.359049000
6	-4.297468000	-1.061220000	1.845939000
6	-2.109564000	-2.069850000	1.341099000
6	-1.473294000	-0.873921000	1.886484000
6	0.732363000	-1.863429000	1.360346000
6	-0.078553000	-0.776671000	1.913067000
6	2.112706000	-1.758755000	1.366387000
6	2.747718000	-0.568351000	1.932666000
6	4.949082000	-1.513814000	1.328740000
6	4.147509000	-0.469271000	1.954714000
6	6.365198000	-1.433621000	1.351365000
6	6.983584000	-0.266365000	1.887633000
6	-6.331806000	-2.479105000	-0.977327000
6	-5.597663000	-2.862526000	0.202444000
6	-3.484275000	-2.412185000	-1.037470000
6	-4.187771000	-2.742644000	0.199558000
6	-2.094511000	-2.294720000	-1.022039000
6	-1.333791000	-2.592597000	0.203796000
6	0.748516000	-2.090786000	-1.040309000
6	0.045266000	-2.469959000	0.201895000
6	2.128981000	-1.987483000	-1.046960000
6	2.881128000	-2.232623000	0.198737000
6	4.964631000	-1.737229000	-1.019035000
6	4.262652000	-2.139700000	0.199203000
6	6.380731000	-1.660630000	-1.036526000
6	7.105651000	-1.848163000	0.190747000
6	-6.484458000	-0.269261000	-1.807344000
6	-5.710118000	-1.481805000	-1.761775000

6	-3.653994000	-0.127175000	-1.816148000
6	-4.275297000	-1.405406000	-1.737880000
6	-2.241256000	-0.016056000	-1.804021000
6	-1.448662000	-1.221428000	-1.774254000
6	0.562088000	0.175513000	-1.906433000
6	-0.053483000	-1.128306000	-1.797511000
6	1.965940000	0.275984000	-1.930169000
6	2.772862000	-0.924425000	-1.819334000
6	4.801699000	0.468812000	-1.913869000
6	4.172766000	-0.829330000	-1.840317000
6	6.229928000	0.569832000	-1.946001000
6	7.007694000	-0.614172000	-1.774380000
1	-7.589319000	-0.011537000	1.677497000
1	-7.613085000	1.742945000	-0.240946000
1	-7.427373000	-2.363613000	1.304442000
1	-7.570055000	-0.343229000	-1.801932000
1	-7.414131000	-2.582360000	-0.994962000
1	7.919184000	2.019446000	1.019923000
1	8.067511000	-0.201596000	1.937358000
1	7.934783000	1.794810000	-1.339989000
1	8.191518000	-1.861820000	0.198935000
1	8.092204000	-0.558476000	-1.821526000
6	-4.265956000	4.387566000	0.586078000
6	-2.911394000	4.339947000	0.624956000
1	-4.794398000	4.871272000	1.403913000
1	-2.377643000	4.805561000	1.446041000
6	-5.057834000	3.782574000	-0.451877000
1	-6.112851000	4.012500000	-0.438304000
1	-4.650285000	3.715305000	-1.452584000
6	-2.134750000	3.568083000	-0.385090000
1	-1.068614000	3.772779000	-0.308813000
1	-2.440044000	3.817159000	-1.405924000

Zero-point correction= 0.621299 (Hartree/Particle)
 Thermal correction to Energy= 0.655693
 Thermal correction to Enthalpy= 0.656637
 Thermal correction to Gibbs Free Energy= 0.566714
 Sum of electronic and zero-point Energies= -2828.278323
 Sum of electronic and thermal Energies= -2828.243929
 Sum of electronic and thermal Enthalpies= -2828.242985
Sum of electronic and thermal Free Energies= -2828.332909
Number of imaginary frequencies = 1 (-400.8332)

Optimized Geometries of [4+2] adduct with different length

(5,0) Adduct of 11.34Å

6	4.679549000	1.356457000	0.206035000
6	3.900941000	0.900009000	1.342148000
6	1.926151000	2.028346000	0.247685000
6	2.491770000	1.040333000	1.285614000

6	0.332514000	2.142904000	0.246196000
6	-0.372261000	1.268877000	1.319414000
6	-2.466720000	1.943984000	0.205771000
6	-1.760643000	1.339181000	1.353313000
6	-3.860052000	2.056005000	0.205970000
6	-4.613792000	1.479956000	1.285090000
6	4.505887000	0.024999000	-1.688971000
6	3.918086000	1.110943000	-1.004511000
6	1.698873000	0.249131000	-1.588030000
6	2.507889000	1.242962000	-0.944935000
6	0.291176000	0.364029000	-1.608227000
6	-0.355763000	1.479858000	-0.980876000
6	-2.527101000	0.564149000	-1.716147000
6	-1.743772000	1.554760000	-1.022644000
6	-3.961121000	0.670190000	-1.751989000
6	-4.597222000	1.686497000	-0.970183000
6	4.331477000	-2.314212000	-1.273916000
6	3.720536000	-1.155520000	-1.841831000
6	1.486647000	-2.173664000	-1.359191000
6	2.298872000	-1.039805000	-1.782049000
6	0.113818000	-2.060833000	-1.352253000
6	-0.505381000	-0.819558000	-1.824128000
6	-2.711151000	-1.806810000	-1.321214000
6	-1.903442000	-0.722973000	-1.868296000
6	-4.121733000	-1.713973000	-1.351165000
6	-4.732907000	-0.522574000	-1.843597000
6	4.315955000	-2.519814000	0.972034000
6	3.570291000	-2.902913000	-0.200287000
6	1.470015000	-2.393498000	1.042675000
6	2.175294000	-2.771579000	-0.198043000
6	0.096607000	-2.280010000	1.036585000
6	-0.663838000	-2.588819000	-0.201678000
6	-2.728490000	-2.019196000	1.009553000
6	-2.033798000	-2.483599000	-0.202517000
6	-4.139561000	-1.931174000	1.034418000
6	-4.869743000	-2.131241000	-0.192039000
6	4.480879000	-0.296604000	1.819662000
6	3.695829000	-1.484587000	1.735335000
6	1.674583000	-0.056569000	1.721051000
6	2.274280000	-1.358747000	1.678970000
6	0.267293000	0.054417000	1.740326000
6	-0.531272000	-1.146671000	1.719309000
6	-2.553061000	0.237350000	1.840791000
6	-1.930270000	-1.056402000	1.758013000
6	-3.987204000	0.336112000	1.874835000
6	-4.758769000	-0.851267000	1.730561000
1	5.590541000	-0.050048000	-1.728546000
1	5.761754000	1.382743000	0.216269000
1	5.405926000	-2.461308000	-1.341944000
1	5.564863000	-0.377877000	1.864412000

1	5.389438000	-2.678668000	1.027412000
6	1.979202000	4.406477000	-0.609141000
6	0.652161000	4.506516000	-0.607592000
1	2.615129000	4.959504000	-1.291635000
1	0.106428000	5.150368000	-1.288534000
6	2.570049000	3.442741000	0.378508000
1	3.651144000	3.376012000	0.271134000
1	2.386778000	3.787541000	1.403894000
6	-0.079596000	3.644366000	0.379856000
1	-1.155979000	3.750385000	0.275257000
1	0.158768000	3.956113000	1.404518000
1	-5.674603000	1.817734000	-1.014529000
1	-5.691907000	1.602017000	1.337088000
1	-5.816993000	-0.452602000	-1.887806000
1	-5.843472000	-0.787691000	1.768753000
1	-5.955568000	-2.147844000	-0.201364000

Zero-point correction= 0.502228 (Hartree/Particle)
 Thermal correction to Energy= 0.528555
 Thermal correction to Enthalpy= 0.529499
 Thermal correction to Gibbs Free Energy= 0.454008
 Sum of electronic and zero-point Energies= -2066.475872
 Sum of electronic and thermal Energies= -2066.449545
 Sum of electronic and thermal Enthalpies= -2066.448601
Sum of electronic and thermal Free Energies= -2066.524093
Number of imaginary frequencies = 0

(5,0) Adduct of 13.49Å

6	5.679755000	1.364600000	0.205783000
6	4.901379000	0.894597000	1.339198000
6	2.919689000	2.016940000	0.246944000
6	3.490070000	1.032497000	1.286175000
6	1.325343000	2.125831000	0.245853000
6	0.621582000	1.255977000	1.327293000
6	-1.473864000	1.927849000	0.205065000
6	-0.763717000	1.320928000	1.356397000
6	-2.848788000	2.024652000	0.204247000
6	-3.614411000	1.477355000	1.323594000
6	-5.708317000	2.103451000	0.190539000
6	-5.032635000	1.585199000	1.346079000
6	5.504445000	0.032944000	-1.706007000
6	4.917637000	1.105499000	-1.003760000
6	2.695097000	0.246178000	-1.598388000
6	3.505289000	1.235912000	-0.946951000
6	1.285431000	0.360411000	-1.620488000
6	0.637665000	1.471119000	-0.990533000
6	-1.528750000	0.558187000	-1.754577000
6	-0.746980000	1.539748000	-1.028059000
6	-2.938731000	0.659498000	-1.782097000
6	-3.597961000	1.691551000	-1.006511000

6	-5.773873000	0.833761000	-1.748395000
6	-5.016034000	1.804328000	-1.030852000
6	5.335376000	-2.293759000	-1.282614000
6	4.719473000	-1.150525000	-1.860626000
6	2.486442000	-2.168497000	-1.355491000
6	3.293924000	-1.039313000	-1.792302000
6	1.108212000	-2.054802000	-1.341222000
6	0.488646000	-0.826920000	-1.840080000
6	-1.716770000	-1.833958000	-1.350615000
6	-0.905649000	-0.735867000	-1.884348000
6	-3.098509000	-1.736698000	-1.363648000
6	-3.738195000	-0.536922000	-1.876962000
6	-5.938999000	-1.479506000	-1.285688000
6	-5.166899000	-0.441094000	-1.907640000
6	5.321024000	-2.501533000	0.981296000
6	4.585081000	-2.868947000	-0.198333000
6	2.470837000	-2.388900000	1.040072000
6	3.180142000	-2.741774000	-0.195725000
6	1.092121000	-2.273580000	1.028321000
6	0.328383000	-2.593665000	-0.201287000
6	-1.733506000	-2.053383000	1.038236000
6	-1.038161000	-2.481528000	-0.200729000
6	-3.115483000	-1.958405000	1.049213000
6	-3.863593000	-2.204430000	-0.195234000
6	-5.955029000	-1.688167000	0.980312000
6	-5.267298000	-2.131833000	-0.198391000
6	5.480712000	-0.292389000	1.835296000
6	4.696239000	-1.483743000	1.752604000
6	2.672088000	-0.062392000	1.730225000
6	3.270772000	-1.361106000	1.688496000
6	1.262602000	0.047122000	1.752147000
6	0.463770000	-1.158572000	1.736457000
6	-1.554454000	0.222837000	1.879483000
6	-0.931347000	-1.073796000	1.775580000
6	-2.964733000	0.318953000	1.904881000
6	-3.763875000	-0.873260000	1.766099000
6	-5.799781000	0.500621000	1.861921000
6	-5.193197000	-0.782491000	1.792547000
1	6.589083000	-0.041364000	-1.746390000
1	6.761833000	1.386834000	0.215209000
1	6.413953000	-2.418440000	-1.332423000
1	6.564751000	-0.372971000	1.879566000
1	6.399076000	-2.633962000	1.020911000
6	2.966312000	4.394128000	-0.610409000
6	1.638895000	4.491618000	-0.605807000
1	3.599685000	4.948849000	-1.293913000
1	1.090254000	5.134372000	-1.285435000
6	3.561004000	3.432805000	0.376633000
1	4.642109000	3.367890000	0.268211000
1	3.377824000	3.776876000	1.402250000

6	0.911486000	3.628231000	0.382943000
1	-0.164682000	3.733656000	0.282304000
1	1.152720000	3.939468000	1.407094000
1	-6.785521000	2.242160000	0.195919000
1	-6.857542000	0.916622000	-1.780344000
1	-6.883948000	0.577381000	1.891316000
1	-7.023486000	-1.470937000	-1.347175000
1	-7.040404000	-1.687844000	1.025941000

Zero-point correction= 0.563904 (Hartree/Particle)
 Thermal correction to Energy= 0.594085
 Thermal correction to Enthalpy= 0.595029
 Thermal correction to Gibbs Free Energy= 0.512747
 Sum of electronic and zero-point Energies= -2447.407435
 Sum of electronic and thermal Energies= -2447.377255
 Sum of electronic and thermal Enthalpies= -2447.376310
Sum of electronic and thermal Free Energies= -2447.458593
Number of imaginary frequencies = 0

(5,0) Adduct of 15.63Å

6	-6.682794000	1.406604000	-0.206432000
6	-5.909480000	0.920337000	-1.337667000
6	-3.914385000	2.023662000	-0.246670000
6	-4.495125000	1.045256000	-1.286860000
6	-2.319487000	2.117766000	-0.245830000
6	-1.622665000	1.243280000	-1.329986000
6	0.479889000	1.901982000	-0.205880000
6	-0.235989000	1.293169000	-1.354050000
6	1.852199000	1.972534000	-0.204017000
6	2.611414000	1.439543000	-1.347505000
6	4.704872000	2.065854000	-0.195096000
6	4.007082000	1.525245000	-1.358185000
6	6.118793000	2.170489000	-0.196292000
6	6.857793000	1.624029000	-1.293505000
6	-6.518887000	0.070301000	1.714638000
6	-5.924058000	1.130131000	1.002066000
6	-3.706773000	0.253962000	1.601538000
6	-4.508437000	1.248077000	0.947375000
6	-2.292704000	0.356428000	1.622420000
6	-1.636673000	1.458860000	0.992814000
6	0.522336000	0.531955000	1.767780000
6	-0.250521000	1.511789000	1.025617000
6	1.928347000	0.621392000	1.796271000
6	2.597055000	1.658537000	1.026441000
6	4.767328000	0.776300000	1.784071000
6	3.992802000	1.746522000	1.039036000
6	6.198561000	0.864160000	1.814818000
6	6.843861000	1.835271000	0.990911000
6	-6.370368000	-2.251855000	1.286918000
6	-5.743880000	-1.120619000	1.870041000

6	-3.519605000	-2.157102000	1.353854000
6	-4.315055000	-1.023504000	1.798693000
6	-2.136707000	-2.052485000	1.335624000
6	-1.506970000	-0.837431000	1.845353000
6	0.692671000	-1.865077000	1.357844000
6	-0.110413000	-0.758837000	1.887795000
6	2.070722000	-1.774800000	1.366155000
6	2.718935000	-0.585544000	1.919934000
6	4.909783000	-1.563782000	1.326085000
6	4.121492000	-0.503640000	1.941436000
6	6.326635000	-1.500947000	1.350861000
6	6.959589000	-0.339605000	1.882575000
6	-6.358054000	-2.460251000	-0.986403000
6	-5.630195000	-2.825138000	0.196975000
6	-3.506234000	-2.376980000	-1.038390000
6	-4.218417000	-2.712420000	0.194564000
6	-2.122770000	-2.270111000	-1.023252000
6	-1.361418000	-2.599054000	0.201042000
6	0.707109000	-2.085711000	-1.044332000
6	0.007569000	-2.489827000	0.199646000
6	2.085515000	-1.997304000	-1.052010000
6	2.835276000	-2.262140000	0.196076000
6	4.923962000	-1.779943000	-1.017198000
6	4.215291000	-2.186486000	0.197524000
6	6.341192000	-1.720905000	-1.034982000
6	7.063579000	-1.925278000	0.191312000
6	-6.498012000	-0.256348000	-1.844282000
6	-5.723799000	-1.455366000	-1.761466000
6	-3.686625000	-0.055160000	-1.733474000
6	-4.294902000	-1.346390000	-1.694365000
6	-2.272967000	0.042569000	-1.754434000
6	-1.485358000	-1.170361000	-1.741170000
6	0.544771000	0.193366000	-1.893915000
6	-0.088008000	-1.098013000	-1.778763000
6	1.950892000	0.277147000	-1.920733000
6	2.741570000	-0.930904000	-1.808622000
6	4.789701000	0.435053000	-1.901909000
6	4.144612000	-0.852629000	-1.826928000
6	6.221011000	0.516915000	-1.931084000
6	6.981432000	-0.677375000	-1.764888000
1	-7.604118000	0.003694000	1.752317000
1	-7.764882000	1.429561000	-0.215074000
1	-7.451563000	-2.357160000	1.327829000
1	-7.582760000	-0.328430000	-1.885694000
1	-7.438990000	-2.570992000	-1.018401000
1	7.924774000	1.943021000	1.021524000
1	8.044508000	-0.288025000	1.927734000
1	7.939076000	1.725729000	-1.330843000
1	8.149217000	-1.950976000	0.200055000
1	8.066863000	-0.632990000	-1.804752000

6	-3.940157000	4.398348000	0.614817000
6	-2.611831000	4.484251000	0.609025000
1	-4.568505000	4.957102000	1.299737000
1	-2.056665000	5.120765000	1.289282000
6	-4.543321000	3.445163000	-0.374600000
1	-5.625128000	3.389462000	-0.267221000
1	-4.355998000	3.788899000	-1.399611000
6	-1.893395000	3.617295000	-0.382563000
1	-0.816428000	3.713264000	-0.284332000
1	-2.134621000	3.931753000	-1.405773000

Zero-point correction= 0.624918 (Hartree/Particle)
 Thermal correction to Energy= 0.659099
 Thermal correction to Enthalpy= 0.660043
 Thermal correction to Gibbs Free Energy= 0.570637
 Sum of electronic and zero-point Energies= -2828.337921
 Sum of electronic and thermal Energies= -2828.303740
 Sum of electronic and thermal Enthalpies= -2828.302796
Sum of electronic and thermal Free Energies= -2828.392202
Number of imaginary frequencies = 0

Optimized Geometries of [5+4] adduct with different length

(5,0) Adduct of 11.34Å

6	-4.464312000	1.670079000	-0.230486000
6	-3.855707000	0.731237000	-1.299978000
6	-1.813607000	1.439649000	-0.198539000
6	-2.432693000	0.835672000	-1.312197000
6	-0.434311000	1.957199000	-0.218192000
6	0.379566000	1.271012000	-1.353205000
6	2.396001000	2.104027000	-0.196012000
6	1.748033000	1.446887000	-1.351176000
6	3.777283000	2.307132000	-0.197833000
6	4.578441000	1.782746000	-1.269645000
6	-4.446367000	-0.158924000	1.591525000
6	-3.875633000	0.946054000	0.994406000
6	-1.610183000	0.157881000	1.755313000
6	-2.457353000	1.039732000	0.998129000
6	-0.213611000	0.353399000	1.736836000
6	0.349081000	1.483067000	1.039861000
6	2.573880000	0.722588000	1.740778000
6	1.718654000	1.660540000	1.041379000
6	3.994445000	0.917663000	1.756770000
6	4.551244000	1.982238000	0.968389000
6	-4.114083000	-2.498754000	1.240983000
6	-3.588630000	-1.313108000	1.812122000
6	-1.296338000	-2.226844000	1.358156000
6	-2.175253000	-1.162831000	1.855648000
6	0.073002000	-2.030217000	1.351901000
6	0.646003000	-0.791183000	1.886910000

6	2.898479000	-1.626206000	1.316784000
6	2.034966000	-0.604721000	1.899608000
6	4.300294000	-1.450894000	1.340934000
6	4.839075000	-0.223854000	1.832810000
6	-4.086205000	-2.699392000	-0.963123000
6	-3.299442000	-3.098612000	0.194935000
6	-1.267963000	-2.439719000	-1.056854000
6	-1.932770000	-2.877084000	0.191356000
6	0.101621000	-2.242012000	-1.052167000
6	0.877079000	-2.488834000	0.190479000
6	2.926074000	-1.833602000	-1.019889000
6	2.245499000	-2.308201000	0.191687000
6	4.328287000	-1.662244000	-1.039507000
6	5.071365000	-1.828562000	0.183830000
6	-4.414732000	-0.457888000	-1.711886000
6	-3.547475000	-1.629321000	-1.718630000
6	-1.566616000	-0.163770000	-1.889717000
6	-2.132408000	-1.482798000	-1.756909000
6	-0.172018000	0.036166000	-1.865008000
6	0.689801000	-1.115968000	-1.784523000
6	2.618001000	0.403865000	-1.856150000
6	2.078683000	-0.931645000	-1.793489000
6	4.038067000	0.595563000	-1.871787000
6	4.882016000	-0.540108000	-1.726111000
1	-5.522701000	-0.312285000	1.546052000
1	-5.553534000	1.604195000	-0.233989000
1	-5.179541000	-2.706855000	1.295284000
1	-5.491004000	-0.608273000	-1.656867000
1	-5.149935000	-2.918383000	-1.006390000
6	-3.088764000	3.859920000	0.588335000
6	-1.753458000	4.038137000	0.592086000
1	-3.616381000	4.283574000	1.440661000
1	-1.355736000	4.581175000	1.445365000
6	-4.007534000	3.190294000	-0.430414000
1	-4.925151000	3.785085000	-0.457865000
1	-3.565885000	3.270867000	-1.425180000
6	-0.695407000	3.517577000	-0.371770000
1	0.245106000	4.051083000	-0.225008000
1	-1.006254000	3.667712000	-1.409309000
1	5.641571000	1.996379000	-1.329687000
1	5.612925000	2.205926000	1.016387000
1	5.960888000	-0.409803000	-1.759636000
1	5.917106000	-0.087083000	1.867608000
1	6.156137000	-1.781484000	0.192054000

Zero-point correction=	0.502995 (Hartree/Particle)
Thermal correction to Energy=	0.529229
Thermal correction to Enthalpy=	0.530173
Thermal correction to Gibbs Free Energy=	0.454971
Sum of electronic and zero-point Energies=	-2066.478376

Sum of electronic and thermal Energies= -2066.452143
Sum of electronic and thermal Enthalpies= -2066.451199
Sum of electronic and thermal Free Energies= -2066.526401
Number of imaginary frequencies = 0

(5,0) Adduct of 13.49Å

6	-5.409654000	1.795628000	-0.228290000
6	-4.835816000	0.836638000	-1.300351000
6	-2.769141000	1.470657000	-0.198268000
6	-3.409075000	0.888391000	-1.311199000
6	-1.369498000	1.928690000	-0.215893000
6	-0.580036000	1.219202000	-1.354595000
6	1.471804000	1.969745000	-0.192369000
6	0.793036000	1.340726000	-1.351242000
6	2.844772000	2.101433000	-0.192237000
6	3.630505000	1.589893000	-1.317687000
6	5.704776000	2.278919000	-0.182091000
6	5.041721000	1.741702000	-1.338813000
6	-5.459243000	-0.033906000	1.591920000
6	-4.848173000	1.050051000	0.997021000
6	-2.612896000	0.177303000	1.750789000
6	-3.426901000	1.091035000	0.997935000
6	-1.206668000	0.321578000	1.734239000
6	-0.603262000	1.430983000	1.045356000
6	1.585730000	0.598781000	1.786241000
6	0.771048000	1.552934000	1.046604000
6	2.987382000	0.740141000	1.801331000
6	3.610078000	1.794716000	1.018070000
6	5.810715000	1.001718000	1.751300000
6	5.021352000	1.950785000	1.039195000
6	-5.211230000	-2.386638000	1.239438000
6	-4.646176000	-1.220362000	1.801976000
6	-2.384610000	-2.214315000	1.352430000
6	-3.222261000	-1.120494000	1.843024000
6	-1.006024000	-2.062778000	1.340999000
6	-0.390196000	-0.853459000	1.894683000
6	1.832264000	-1.778440000	1.342642000
6	1.001383000	-0.718986000	1.912338000
6	3.213728000	-1.644088000	1.352113000
6	3.820819000	-0.434099000	1.880447000
6	6.046875000	-1.302375000	1.277441000
6	5.245005000	-0.294424000	1.909533000
6	-5.190807000	-2.586642000	-0.968155000
6	-4.419796000	-3.017364000	0.191833000
6	-2.363657000	-2.425454000	-1.056980000
6	-3.045662000	-2.840782000	0.188127000
6	-0.985090000	-2.272016000	-1.047363000
6	-0.214941000	-2.560235000	0.188550000
6	1.853315000	-1.987988000	-1.045689000
6	1.154447000	-2.412087000	0.188644000

6	3.234918000	-1.855141000	-1.053205000
6	3.991584000	-2.082122000	0.185390000
6	6.066803000	-1.501190000	-0.989816000
6	5.394326000	-1.967221000	0.187695000
6	-5.438318000	-0.330550000	-1.712188000
6	-4.616506000	-1.532251000	-1.710894000
6	-2.580651000	-0.142003000	-1.886398000
6	-3.190741000	-1.436461000	-1.747853000
6	-1.176193000	0.007054000	-1.862735000
6	-0.357502000	-1.177443000	-1.793556000
6	1.619378000	0.274977000	-1.901822000
6	1.034062000	-1.045620000	-1.806341000
6	3.020160000	0.413575000	-1.916176000
6	3.853255000	-0.755571000	-1.774962000
6	5.842575000	0.684730000	-1.860447000
6	5.277550000	-0.620120000	-1.801438000
1	-6.540478000	-0.147584000	1.544211000
1	-6.500584000	1.770812000	-0.232137000
1	-6.285145000	-2.548850000	1.286407000
1	-6.519299000	-0.441379000	-1.654106000
1	-6.263442000	-2.758891000	-1.006032000
6	-3.952146000	3.931786000	0.593350000
6	-2.610810000	4.058765000	0.595517000
1	-4.462967000	4.376034000	1.445414000
1	-2.191471000	4.587470000	1.447471000
6	-4.895737000	3.298356000	-0.425866000
1	-5.790841000	3.926656000	-0.452045000
1	-4.451947000	3.363372000	-1.420775000
6	-1.574738000	3.498353000	-0.369653000
1	-0.613134000	3.993657000	-0.223121000
1	-1.879621000	3.660996000	-1.407099000
1	6.774878000	2.463112000	-0.189311000
1	6.923379000	0.797562000	-1.895151000
1	6.890851000	1.121031000	1.786550000
1	7.151703000	-1.465314000	-1.033771000
1	7.130851000	-1.258394000	1.333901000

Zero-point correction= 0.564871 (Hartree/Particle)
 Thermal correction to Energy= 0.594934
 Thermal correction to Enthalpy= 0.595879
 Thermal correction to Gibbs Free Energy= 0.513905
 Sum of electronic and zero-point Energies= -2447.412169
 Sum of electronic and thermal Energies= -2447.382106
 Sum of electronic and thermal Enthalpies= -2447.381161
Sum of electronic and thermal Free Energies= -2447.463135
Number of imaginary frequencies = 0

(5,0) Adduct of 15.63Å

6	-6.390565000	1.886785000	-0.226471000
6	-5.837613000	0.917044000	-1.300744000

6	-3.757190000	1.506833000	-0.197552000
6	-4.412433000	0.937596000	-1.312162000
6	-2.346362000	1.931025000	-0.214070000
6	-1.571925000	1.201686000	-1.349833000
6	0.497569000	1.913883000	-0.190462000
6	-0.195008000	1.289781000	-1.344457000
6	1.870323000	1.997363000	-0.188740000
6	2.642384000	1.489817000	-1.340640000
6	4.720808000	2.156961000	-0.183208000
6	4.031862000	1.599998000	-1.349200000
6	6.126997000	2.288345000	-0.185403000
6	6.879669000	1.758001000	-1.282776000
6	-6.481448000	0.052836000	1.588012000
6	-5.845730000	1.127111000	0.998103000
6	-3.632241000	0.194026000	1.729987000
6	-4.425665000	1.137106000	0.998531000
6	-2.216678000	0.308676000	1.714829000
6	-1.590978000	1.412665000	1.045649000
6	0.578412000	0.530756000	1.793472000
6	-0.213090000	1.500508000	1.045164000
6	1.979575000	0.641292000	1.811719000
6	2.626139000	1.698746000	1.043702000
6	4.810978000	0.847294000	1.789055000
6	4.015655000	1.810617000	1.052838000
6	6.238488000	0.962908000	1.816093000
6	6.864152000	1.958237000	0.997340000
6	-6.286243000	-2.308843000	1.236457000
6	-5.697095000	-1.151516000	1.788883000
6	-3.454579000	-2.202753000	1.349799000
6	-4.267217000	-1.085338000	1.828430000
6	-2.072157000	-2.077082000	1.333922000
6	-1.431033000	-0.880116000	1.882913000
6	0.774871000	-1.856528000	1.346041000
6	-0.032813000	-0.774817000	1.900586000
6	2.155765000	-1.744236000	1.350208000
6	2.787476000	-0.554716000	1.918135000
6	4.994725000	-1.486210000	1.314334000
6	4.189754000	-0.447401000	1.937910000
6	6.412134000	-1.397183000	1.338466000
6	7.021686000	-0.224416000	1.872729000
6	-6.270472000	-2.507113000	-0.971625000
6	-5.507007000	-2.958502000	0.188256000
6	-3.437974000	-2.412863000	-1.060033000
6	-4.129514000	-2.813633000	0.184973000
6	-2.056006000	-2.285048000	-1.046447000
6	-1.290358000	-2.597946000	0.186254000
6	0.791810000	-2.066187000	-1.052862000
6	0.082105000	-2.464682000	0.185471000
6	2.172480000	-1.954954000	-1.056173000
6	2.927879000	-2.211905000	0.184179000

6	5.010879000	-1.691914000	-1.026492000
6	4.310512000	-2.111235000	0.185096000
6	6.428095000	-1.606505000	-1.045012000
6	7.154039000	-1.804897000	0.178194000
6	-6.466489000	-0.239950000	-1.708367000
6	-5.674227000	-1.457300000	-1.701109000
6	-3.607520000	-0.118626000	-1.863272000
6	-4.242604000	-1.395896000	-1.736991000
6	-2.192732000	0.000461000	-1.840361000
6	-1.405291000	-1.199522000	-1.784644000
6	0.605237000	0.208018000	-1.906614000
6	-0.007185000	-1.097266000	-1.797315000
6	2.005748000	0.315084000	-1.923830000
6	2.813787000	-0.881068000	-1.813466000
6	4.836076000	0.525180000	-1.897439000
6	4.215620000	-0.776797000	-1.831137000
6	6.263689000	0.635663000	-1.924632000
6	7.046397000	-0.542868000	-1.765554000
1	-7.564851000	-0.036407000	1.538241000
1	-7.481683000	1.886706000	-0.230658000
1	-7.363132000	-2.449233000	1.285100000
1	-7.549517000	-0.326329000	-1.647623000
1	-7.346260000	-2.657656000	-1.011428000
1	7.940327000	2.102157000	1.036529000
1	8.105669000	-0.150828000	1.911387000
1	7.956596000	1.893448000	-1.331167000
1	8.240131000	-1.801422000	0.184947000
1	8.130816000	-0.475764000	-1.802587000
6	-4.884834000	3.987688000	0.599391000
6	-3.540953000	4.085214000	0.600381000
1	-5.385372000	4.441417000	1.452493000
1	-3.109156000	4.604307000	1.451976000
6	-5.842482000	3.377956000	-0.421143000
1	-6.723015000	4.026423000	-0.446349000
1	-5.397346000	3.434359000	-1.415955000
6	-2.518158000	3.504163000	-0.367035000
1	-1.545059000	3.976275000	-0.220172000
1	-2.819577000	3.675605000	-1.404134000

Zero-point correction=	0.626168 (Hartree/Particle)
Thermal correction to Energy=	0.660167
Thermal correction to Enthalpy=	0.661111
Thermal correction to Gibbs Free Energy=	0.572203
Sum of electronic and zero-point Energies=	-2828.344588
Sum of electronic and thermal Energies=	-2828.310589
Sum of electronic and thermal Enthalpies=	-2828.309645
Sum of electronic and thermal Free Energies=	-2828.398553
Number of imaginary frequencies = 0	