

Supplementary Information

Edge effects, electronic arrangement, and geometry patterns on finite-length carbon nanotubes

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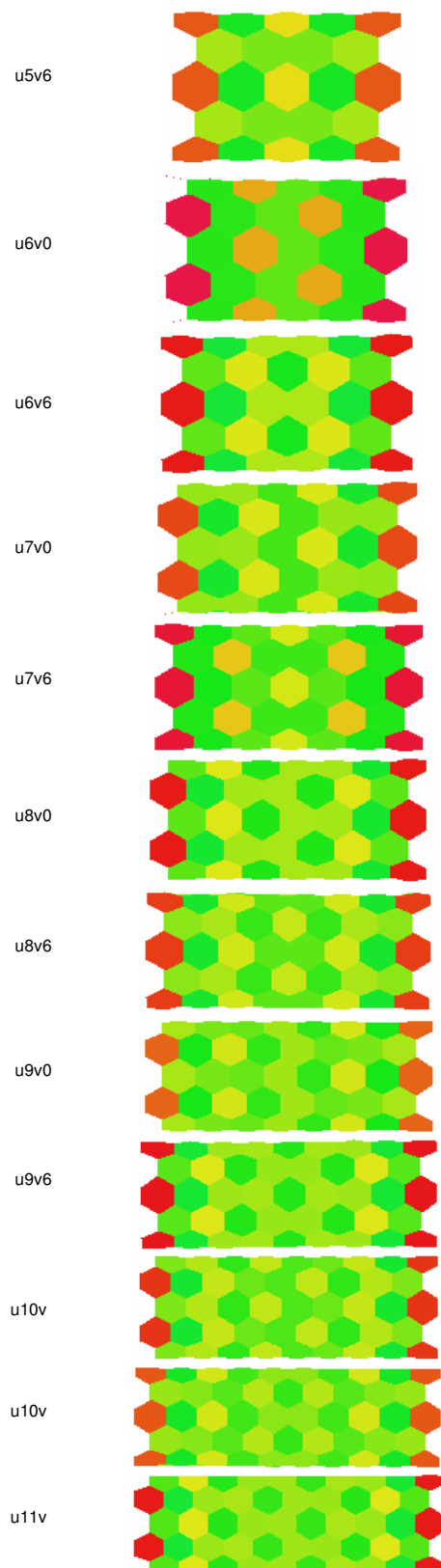
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Ciencias. c/Severo Ochoa s/n. Universidad de Granada. 18071-Granada. (Spain)

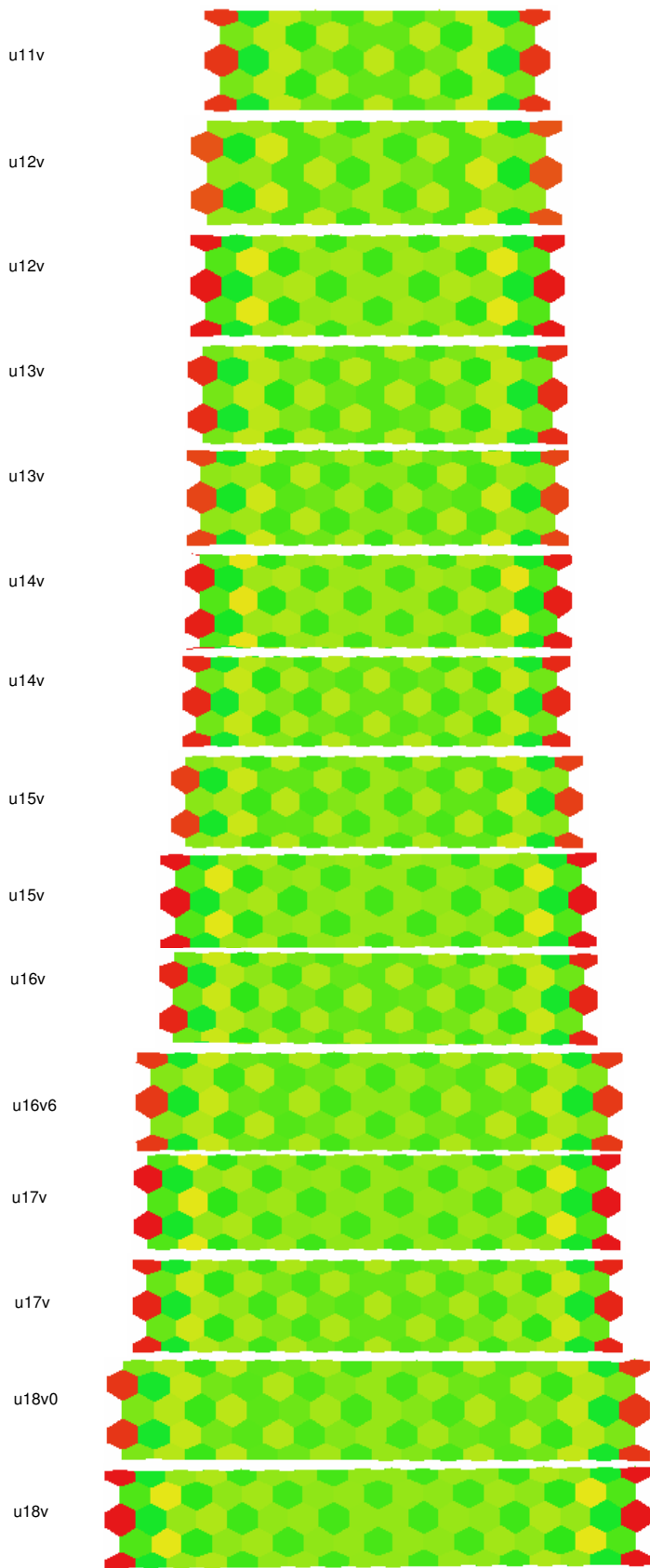
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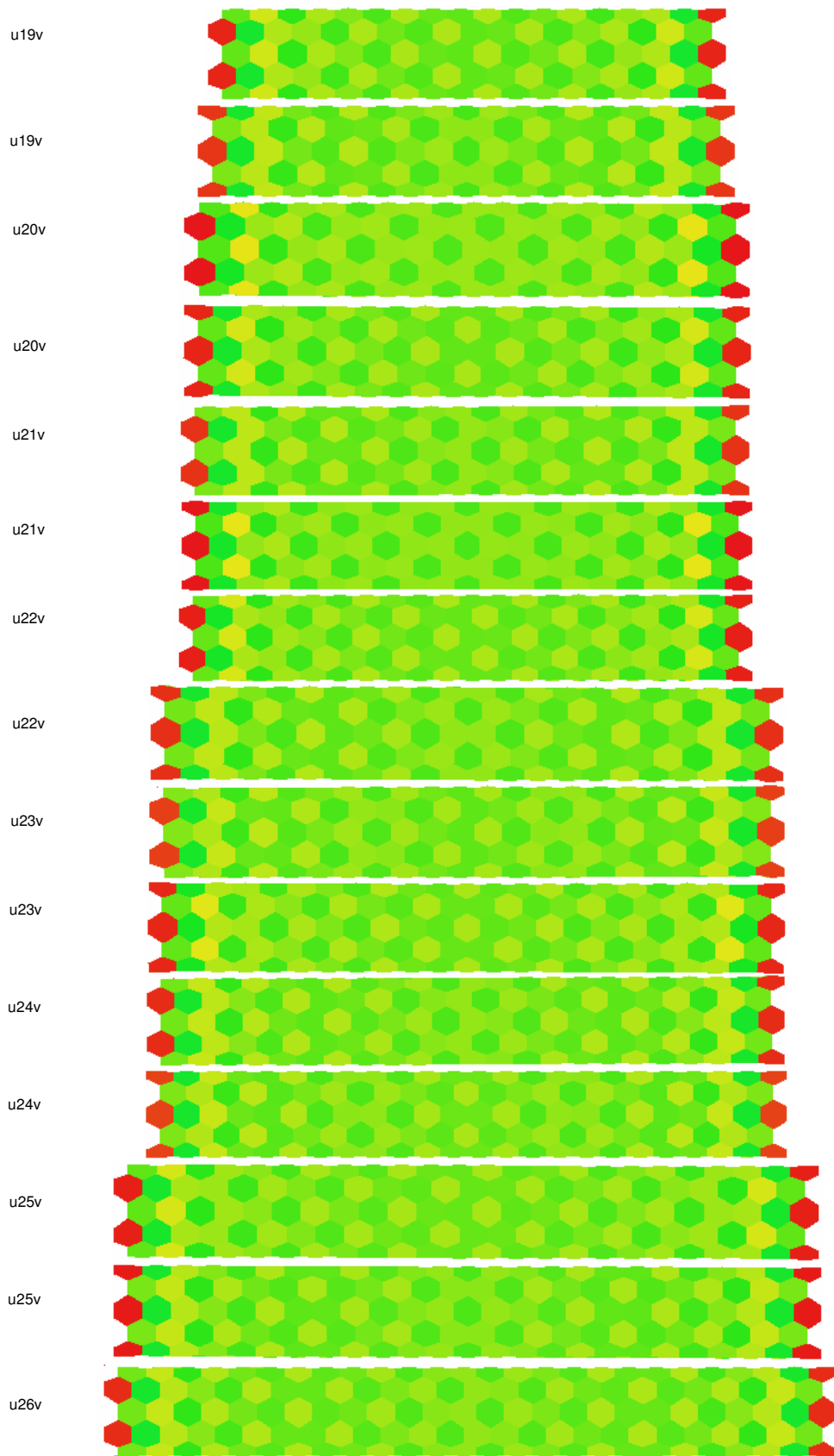
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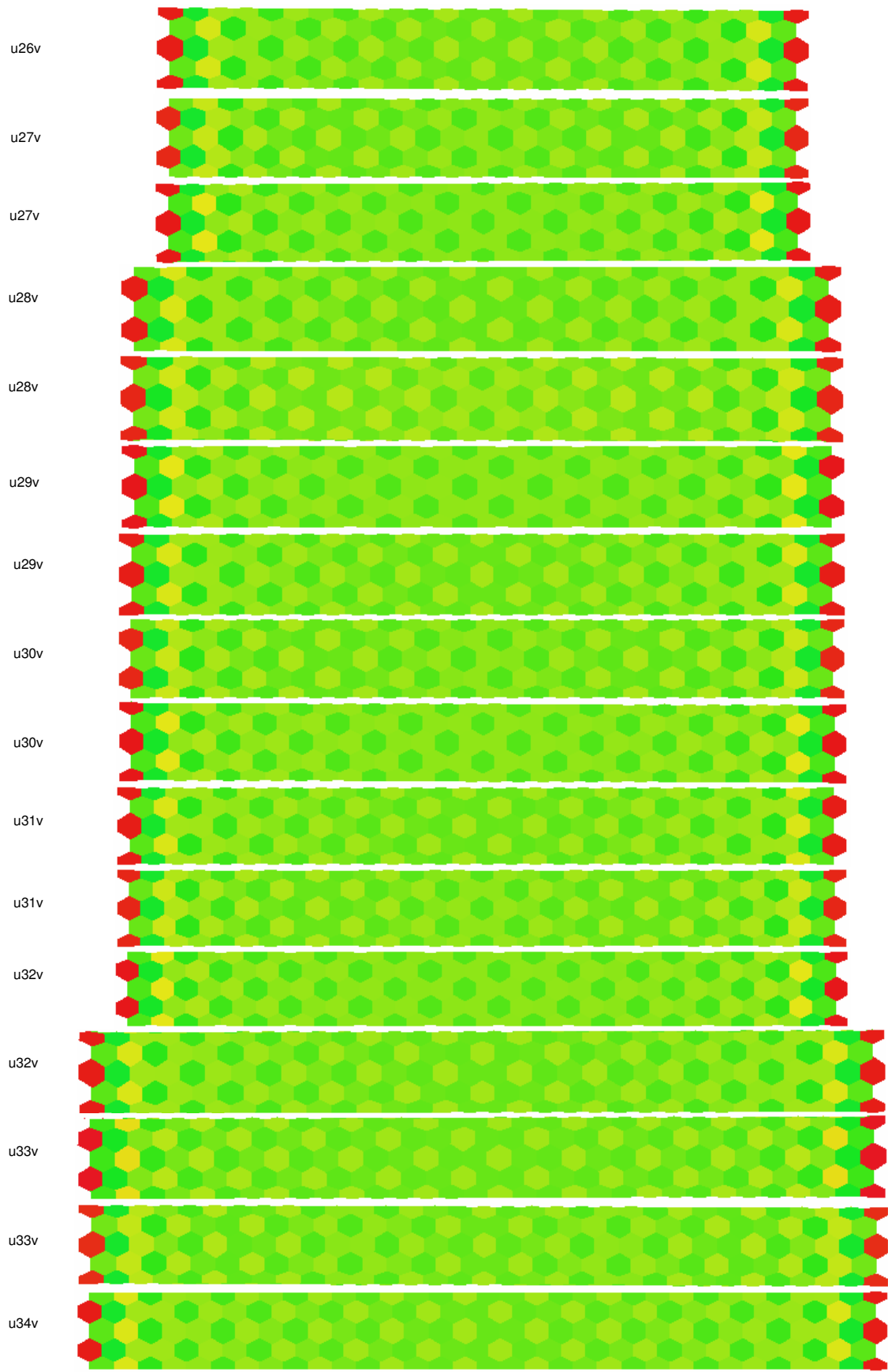
- 1) **TubeAnalyzer plots**.....p S2-S7
- 2) **XYZ and energies for the structures studied**p S8-S854

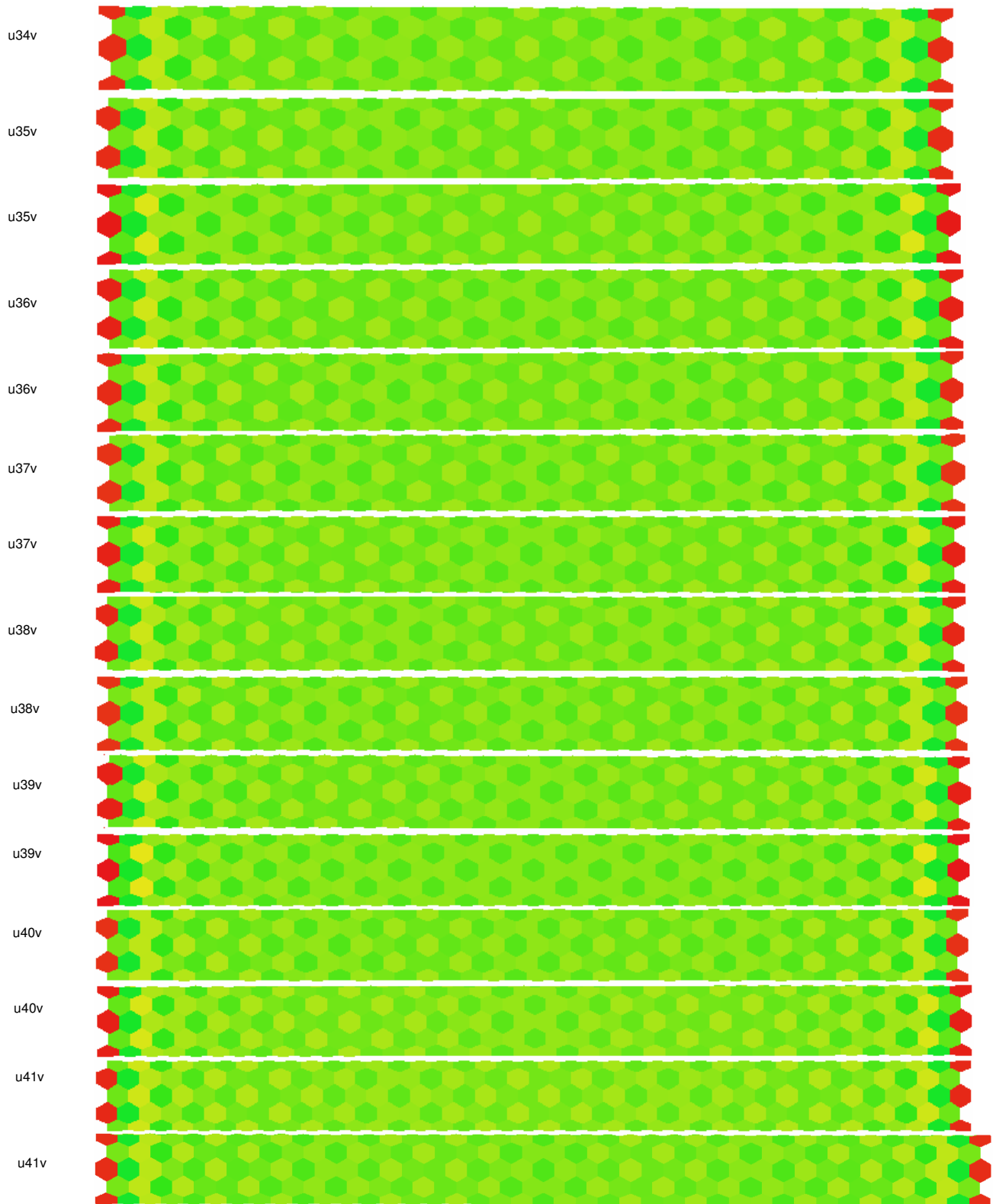
I. TubeAnalyzer MBL plots for (6,6) nanotube:



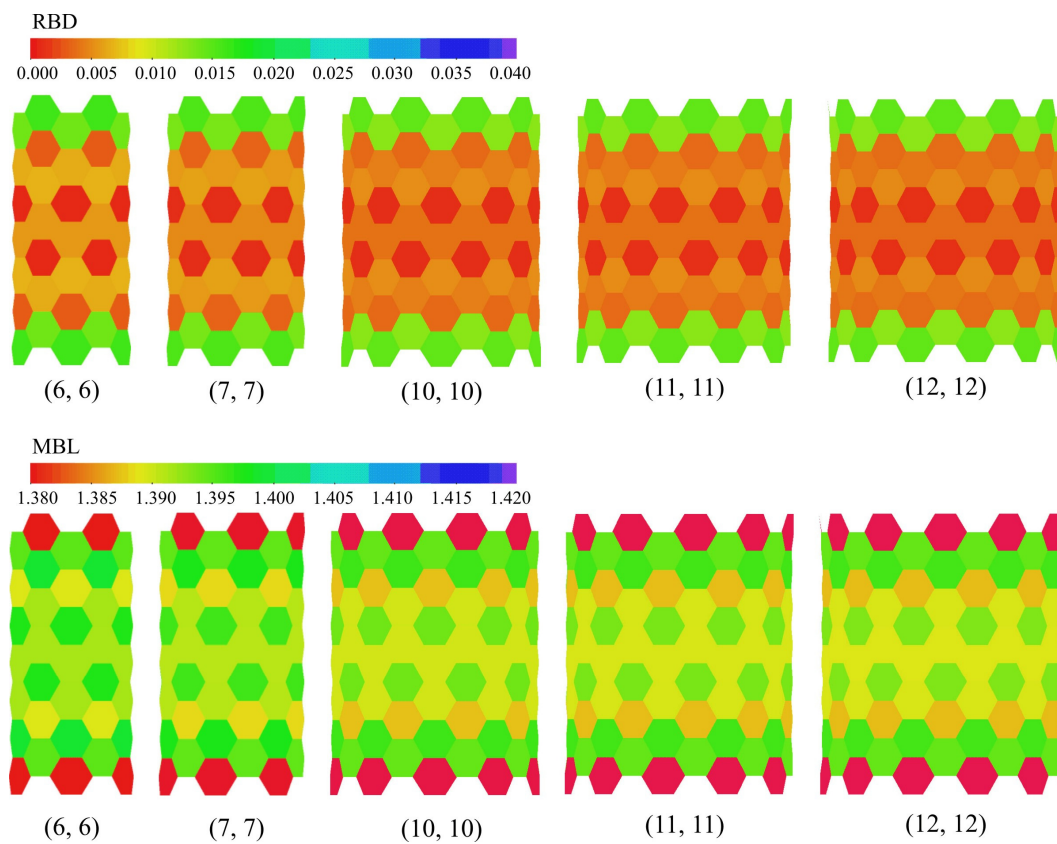








I. TubeAnalyzer RBD and MBL plots for diameter increasing CNTs:



II. Optimized CNTs geometries and Total Calculated Energies (B3LYP/STO-3G):

Nanotube (6,6) u05v6s
B3LYP/STO-3G Energy: -4983.433839

C	-3.463242720	2.487988130	-6.225240610
C	-2.487988130	3.463242720	-6.225240610
C	0.423039560	4.243250240	-6.225240610
C	1.755262110	3.886282280	-6.225240610
C	3.886282280	1.755262110	-6.225240610
C	4.243250240	0.423039560	-6.225240610
C	3.463242720	-2.487988130	-6.225240610
C	2.487988130	-3.463242720	-6.225240610
C	-0.423039560	-4.243250240	-6.225240610
C	-1.755262110	-3.886282280	-6.225240610
C	-3.886282280	-1.755262110	-6.225240610
C	-4.243250240	-0.423039560	-6.225240610
C	-1.776994790	3.809426990	-5.005137710
C	-0.365790860	4.187557940	-5.005137710
C	2.410563150	3.443636120	-5.005137710
C	3.443636120	2.410563150	-5.005137710
C	4.187557940	-0.365790860	-5.005137710
C	3.809426990	-1.776994790	-5.005137710
C	1.776994790	-3.809426990	-5.005137710
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C	-2.410563150	-3.443636120	-5.005137710
C	-3.443636120	-2.410563150	-5.005137710
C	-4.187557940	0.365790860	-5.005137710
C	-3.809426990	1.776994790	-5.005137710
C	0.358195310	4.145473630	-3.763545780
C	1.762530580	3.769183120	-3.763545780
C	3.769183120	1.762530580	-3.763545780
C	4.145473630	0.358195310	-3.763545780
C	3.410987820	-2.382943050	-3.763545780
C	2.382943050	-3.410987820	-3.763545780
C	-0.358195310	-4.145473630	-3.763545780
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C	-3.769183120	-1.762530580	-3.763545780
C	-4.145473630	-0.358195310	-3.763545780
C	-3.410987820	2.382943050	-3.763545780
C	-2.382943050	3.410987820	-3.763545780
C	2.383264470	3.393157960	-2.505401370
C	3.393157960	2.383264470	-2.505401370
C	4.130193230	-0.367388600	-2.505401370
C	3.760546560	-1.746928750	-2.505401370
C	1.746928750	-3.760546560	-2.505401370
C	0.367388600	-4.130193230	-2.505401370
C	-2.383264470	-3.393157960	-2.505401370
C	-3.393157960	-2.383264470	-2.505401370
C	-4.130193230	0.367388600	-2.505401370
C	-3.760546560	1.746928750	-2.505401370
C	-1.746928750	3.760546560	-2.505401370
C	-0.367388600	4.130193230	-2.505401370
C	3.771475750	1.754914270	-1.246772190
C	4.143650940	0.365937540	-1.246772190
C	3.405538210	-2.388736680	-1.246772190
C	2.388736680	-3.405538210	-1.246772190
C	-0.365937540	-4.143650940	-1.246772190
C	-1.754914270	-3.771475750	-1.246772190
C	-3.771475750	-1.754914270	-1.246772190
C	-4.143650940	-0.365937540	-1.246772190
C	-3.405538210	2.388736680	-1.246772190
C	-2.388736680	3.405538210	-1.246772190
C	0.365937540	4.143650940	-1.246772190
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C	-3.418245240	-2.391628790	0.000000000
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C	-1.764472810	3.780333910	0.000000000
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C	3.418245240	2.391628790	0.000000000
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C	2.388736680	-3.405538210	1.246772190
C	-0.365937540	-4.143650940	1.246772190
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C	-3.771475750	-1.754914270	1.246772190
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C	-2.388736680	3.405538210	1.246772190
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C	3.771475750	1.754914270	1.246772190
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C	-3.393157960	-2.383264470	2.505401370
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C	3.393157960	2.383264470	2.505401370
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C	-2.382943050	3.410987820	3.763545780
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C	2.382943050	-3.410987820	3.763545780
C	-2.410563150	-3.443636120	5.005137710
C	-3.443636120	-2.410563150	5.005137710
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C	-1.776994790	3.809426990	5.005137710
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C	-4.243250240	-0.423039560	6.225240610
C	-3.463242720	2.487988130	6.225240610
C	-2.487988130	3.463242720	6.225240610
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C	3.886282280	1.755262110	6.225240610
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C	-1.755262110	-3.886282280	6.225240610
H	-3.895533520	2.160326070	-7.179354400
H	-2.160326070	3.895533520	-7.179354400
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H	3.818664010	2.293467960	-7.179354400
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H	3.895533520	-2.160326070	-7.179354400
H	2.160326070	-3.895533520	-7.179354400
H	0.076869510	-4.453794020	-7.179354400
H	-2.293467960	-3.818664010	-7.179354400
H	-3.818664010	-2.293467960	-7.179354400
H	-4.453794020	0.076869510	-7.179354400
H	-3.818664010	-2.293467960	7.179354400
H	-4.453794020	0.076869510	7.179354400
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H	-2.160326070	3.895533520	7.179354400
H	-0.076869510	4.453794020	7.179354400
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H	3.818664010	2.293467960	7.179354400
H	4.453794020	-0.076869510	7.179354400
H	3.895533520	-2.160326070	7.179354400
H	2.160326070	-3.895533520	7.179354400
H	0.076869510	-4.453794020	7.179354400
H	-2.293467960	-3.818664010	7.179354400

Nanotube (6,6) u06v0s
B3LYP/STO-3G Energy: -5435.207477

H	-2.288459000	-3.792341000	7.783333000
C	-1.763549000	-3.887482000	6.824554000
H	2.137931000	-3.873130000	7.783983000
C	2.485191000	-3.468073000	6.825179000
H	4.427636000	-0.083304000	7.783224000
C	4.248600000	0.419074000	6.824368000
H	2.288459000	3.792341000	7.783333000
C	1.763549000	3.887482000	6.824554000
H	-2.137931000	3.873130000	7.783983000
C	-2.485191000	3.468073000	6.825179000
H	-4.427636000	0.083304000	7.783224000
C	-4.248600000	-0.419074000	6.824368000
C	-0.419645000	-4.244933000	6.824694000
C	0.359380000	-4.201144000	5.615869000
C	3.469117000	-2.485341000	6.825060000
C	3.821438000	-1.789616000	5.615943000
C	3.890570000	1.762823000	6.824231000
C	3.463922000	2.415883000	5.615319000
C	0.419645000	4.244933000	6.824694000
C	-0.359380000	4.201144000	5.615869000
C	-3.469117000	2.485341000	6.825060000
C	-3.821438000	1.789616000	5.615943000
C	-3.890570000	-1.762823000	6.824231000
C	-3.463922000	-2.415883000	5.615319000
C	1.789219000	-3.819928000	5.616095000
C	2.385715000	-3.409725000	4.376575000
C	4.204000000	-0.360148000	5.615626000
C	4.145443000	0.361222000	4.376009000
C	2.416893000	3.461689000	5.615488000
C	1.761963000	3.770523000	4.376108000
C	-1.789219000	3.819928000	5.616095000
C	-2.385715000	3.409725000	4.376575000
C	-4.204000000	0.360148000	5.615626000
C	-4.145443000	-0.361222000	4.376009000
C	-2.416893000	-3.461689000	5.615488000
C	-1.761963000	-3.770523000	4.376108000
C	3.410424000	-2.385702000	4.376494000
C	3.768979000	-1.753909000	3.113020000
C	3.773259000	1.761271000	4.375905000

C	3.405724000	2.388160000	3.112515000
C	0.361987000	4.142719000	4.376257000
C	-0.364897000	4.137594000	3.113027000
C	-3.410424000	2.385702000	4.376494000
C	-3.768979000	1.753909000	3.113020000
C	-3.773259000	-1.761271000	4.375905000
C	-3.405724000	-2.388160000	3.112515000
C	-0.361987000	-4.142719000	4.376257000
C	0.364897000	-4.137594000	3.113027000
C	4.139559000	-0.365606000	3.112760000
C	4.161405000	0.359956000	1.869429000
C	2.389048000	3.403803000	3.112607000
C	1.770355000	3.784147000	1.869452000
C	-1.753601000	3.768168000	3.113190000
C	-2.393687000	3.425236000	1.870024000
C	-4.139559000	0.365606000	3.112760000
C	-4.161405000	-0.359956000	1.869429000
C	-2.389048000	-3.403803000	3.112607000
C	-1.770355000	-3.784147000	1.869452000
C	1.753601000	-3.768168000	3.113190000
C	2.393687000	-3.425236000	1.870024000
C	3.786248000	1.769769000	1.869268000
C	3.418693000	2.395856000	0.627773000
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C	-0.365570000	4.154248000	0.628333000
C	-3.425567000	2.393812000	1.869934000
C	-3.783233000	1.762300000	0.628359000
C	-3.786248000	-1.769769000	1.869268000
C	-3.418693000	-2.395856000	0.627773000
C	-0.360641000	-4.159460000	1.869683000
C	0.365570000	-4.154248000	0.628333000
C	3.425567000	-2.393812000	1.869934000
C	3.783233000	-1.762300000	0.628359000
C	2.396566000	3.417243000	0.627850000
C	1.762052000	3.781969000	-0.628372000
C	-1.761963000	3.782923000	0.628524000
C	-2.396463000	3.418371000	-0.627773000
C	-4.155503000	0.366235000	0.628097000
C	-4.155445000	-0.365299000	-0.628319000
C	-2.396566000	-3.417243000	0.627850000
C	-1.762052000	-3.781969000	-0.628372000
C	1.761963000	-3.782923000	0.628524000
C	2.396463000	-3.418371000	-0.627773000
C	4.155503000	-0.366235000	0.628097000
C	4.155445000	0.365299000	-0.628319000
C	0.365956000	4.154158000	-0.628111000
C	-0.360232000	4.160163000	-1.869469000
C	-3.418312000	2.396710000	-0.627839000
C	-3.785454000	1.770612000	-1.869407000
C	-3.783563000	-1.761538000	-0.628522000
C	-3.425567000	-2.393064000	-1.870030000
C	-0.365956000	-4.154158000	-0.628111000
C	0.360232000	-4.160163000	-1.869469000
C	3.418312000	-2.396710000	-0.627839000
C	3.785454000	-1.770612000	-1.869407000
C	3.783563000	1.761538000	-0.628522000
C	3.425567000	2.393064000	-1.870030000
C	-1.770206000	3.785590000	-1.869285000
C	-2.388836000	3.405372000	-3.112512000
C	-4.160852000	0.360930000	-1.869634000
C	-4.138895000	-0.364595000	-3.112962000
C	-2.393656000	-3.424461000	-1.869967000
C	-1.753641000	-3.767595000	-3.113089000
C	1.770206000	-3.785590000	-1.869285000
C	2.388836000	-3.405372000	-3.112512000
C	4.160852000	-0.360930000	-1.869634000
C	4.138895000	0.364595000	-3.112962000
C	2.393656000	3.424461000	-1.869967000
C	1.753641000	3.767595000	-3.113089000
C	-3.404970000	2.389196000	-3.112553000

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C	-3.768873000	-1.753129000	-3.113170000
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C	0.361562000	-4.144028000	-4.376091000
C	3.404970000	-2.389196000	-3.112553000
C	3.772015000	-1.762251000	-4.376009000
C	3.768873000	1.753129000	-3.113170000
C	3.410117000	2.384978000	-4.376593000
C	0.365298000	4.138091000	-3.112835000
C	-0.361562000	4.144028000	-4.376091000
C	-4.144302000	0.362315000	-4.376152000
C	-4.202716000	-0.359020000	-5.615758000
C	-2.385547000	-3.409148000	-4.376560000
C	-1.789299000	-3.819817000	-5.616053000
C	1.761795000	-3.772498000	-4.375944000
C	2.416660000	-3.463471000	-5.615319000
C	4.144302000	-0.362315000	-4.376152000
C	4.202716000	0.359020000	-5.615758000
C	2.385547000	3.409148000	-4.376560000
C	1.789299000	3.819817000	-5.616053000
C	-1.761795000	3.772498000	-4.375944000
C	-2.416660000	3.463471000	-5.615319000
C	-3.820728000	-1.788645000	-5.616069000
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C	0.419423000	-4.246874000	-6.824491000
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C	3.889451000	-1.763955000	-6.824395000
C	3.820728000	1.788645000	-5.616069000
C	3.468412000	2.484262000	-6.825214000
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C	-0.419423000	4.246874000	-6.824491000
C	-3.463104000	2.417086000	-5.615395000
C	-3.889451000	1.763955000	-6.824395000
C	-2.485118000	-3.467631000	-6.825155000
H	-2.138320000	-3.873007000	-7.783951000
C	1.763358000	-3.889520000	-6.824300000
H	2.288380000	-3.794330000	-7.783003000
C	4.246999000	-0.420086000	-6.824526000
H	4.425623000	0.082485000	-7.783338000
C	2.485118000	3.467631000	-6.825155000
H	2.138320000	3.873007000	-7.783951000
C	-1.763358000	3.889520000	-6.824300000
H	-2.288380000	3.794330000	-7.783003000
C	-4.246999000	0.420086000	-6.824526000
H	-4.425623000	-0.082485000	-7.783338000
H	0.082986000	-4.423212000	7.783542000
H	3.874811000	-2.138795000	7.783811000
H	3.795312000	2.287810000	7.782945000
H	-0.082986000	4.423212000	7.783542000
H	-3.874811000	2.138795000	7.783811000
H	-3.795312000	-2.287810000	7.782945000
H	-3.873611000	-2.137108000	-7.783997000
H	-0.083021000	-4.425477000	-7.783395000
H	3.794568000	-2.288955000	-7.783148000
H	3.873611000	2.137108000	-7.783997000
H	0.083021000	4.425477000	-7.783395000
H	-3.794568000	2.288955000	-7.783148000

Nanotube (6,6) u06v6s
B3LYP/STO-3G Energy: -5886.997143

H	-1.226575000	-4.273198000	8.421337000
C	-0.692555000	-4.213496000	7.464549000
H	3.087411000	-3.198844000	8.421337000
C	3.302717000	-2.706518000	7.464549000
H	4.313986000	1.074354000	8.421337000

C	3.995272000	1.506978000	7.464549000
H	1.226575000	4.273198000	8.421337000
C	0.692555000	4.213496000	7.464549000
H	-3.087411000	3.198844000	8.421337000
C	-3.302717000	2.706518000	7.464549000
H	-4.313986000	-1.074354000	8.421337000
C	-3.995272000	-1.506978000	7.464549000
C	0.692555000	-4.213496000	7.464549000
C	1.437270000	-3.962063000	6.250344000
C	3.995272000	-1.506978000	7.464549000
C	4.149882000	-0.736319000	6.250344000
C	3.302717000	2.706518000	7.464549000
C	2.712612000	3.225744000	6.250344000
C	-0.692555000	4.213496000	7.464549000
C	-1.437270000	3.962063000	6.250344000
C	-3.995272000	1.506978000	7.464549000
C	-4.149882000	0.736319000	6.250344000
C	-3.302717000	-2.706518000	7.464549000
C	-2.712612000	-3.225744000	6.250344000
C	2.712612000	-3.225744000	6.250344000
C	3.186567000	-2.678015000	5.010824000
C	4.149882000	0.736319000	6.250344000
C	3.912513000	1.420640000	5.010824000
C	1.437270000	3.962063000	6.250344000
C	0.725946000	4.098656000	5.010824000
C	-2.712612000	3.225744000	6.250344000
C	-3.186567000	2.678015000	5.010824000
C	-4.149882000	-0.736319000	6.250344000
C	-3.912513000	-1.420640000	5.010824000
C	-1.437270000	-3.962063000	6.250344000
C	-0.725946000	-4.098656000	5.010824000
C	3.912513000	-1.420640000	5.010824000
C	4.087972000	-0.715299000	3.748526000
C	3.186567000	2.678015000	5.010824000
C	2.663453000	3.182638000	3.748526000
C	-0.725946000	4.098656000	5.010824000
C	-1.424519000	3.897937000	3.748526000
C	-3.912513000	1.420640000	5.010824000
C	-4.087972000	0.715299000	3.748526000
C	-3.186567000	-2.678015000	5.010824000
C	-2.663453000	-3.182638000	3.748526000
C	0.725946000	-4.098656000	5.010824000
C	1.424519000	-3.897937000	3.748526000
C	4.087972000	0.715299000	3.748526000
C	3.918464000	1.424636000	2.495999000
C	1.424519000	3.897937000	3.748526000
C	0.725461000	4.105808000	2.495999000
C	-2.663453000	3.182638000	3.748526000
C	-3.193003000	2.681171000	2.495999000
C	-4.087972000	-0.715299000	3.748526000
C	-3.918464000	-1.424636000	2.495999000
C	-1.424519000	-3.897937000	3.748526000
C	-0.725461000	-4.105808000	2.495999000
C	2.663453000	-3.182638000	3.748526000
C	3.193003000	-2.681171000	2.495999000
C	3.193003000	2.681171000	2.495999000
C	2.682803000	3.196502000	1.254199000
C	-0.725461000	4.105808000	2.495999000
C	-1.426850000	3.921627000	1.254199000
C	-3.918464000	1.424636000	2.495999000
C	-4.109654000	0.725125000	1.254199000
C	-3.193003000	-2.681171000	2.495999000
C	-2.682803000	-3.196502000	1.254199000
C	0.725461000	-4.105808000	2.495999000
C	1.426850000	-3.921627000	1.254199000
C	3.918464000	-1.424636000	2.495999000
C	4.109654000	-0.725125000	1.254199000
C	1.426850000	3.921627000	1.254199000
C	0.718366000	4.103344000	0.000000000
C	-2.682803000	3.196502000	1.254199000

C	-3.194417000	2.673796000	0.000000000
C	-4.109654000	-0.725125000	1.254199000
C	-3.912784000	-1.429549000	0.000000000
C	-1.426850000	-3.921627000	1.254199000
C	-0.718366000	-4.103344000	0.000000000
C	2.682803000	-3.196502000	1.254199000
C	3.194417000	-2.673796000	0.000000000
C	4.109654000	0.725125000	1.254199000
C	3.912784000	1.429549000	0.000000000
C	-0.718366000	4.103344000	0.000000000
C	-1.426850000	3.921627000	-1.254199000
C	-3.912784000	1.429549000	0.000000000
C	-4.109654000	0.725125000	-1.254199000
C	-3.194417000	-2.673796000	0.000000000
C	-2.682803000	-3.196502000	-1.254199000
C	0.718366000	-4.103344000	0.000000000
C	1.426850000	-3.921627000	-1.254199000
C	3.912784000	-1.429549000	0.000000000
C	4.109654000	-0.725125000	-1.254199000
C	3.194417000	2.673796000	0.000000000
C	2.682803000	3.196502000	-1.254199000
C	-2.682803000	3.196502000	-1.254199000
C	-3.193003000	2.681171000	-2.495999000
C	-4.109654000	-0.725125000	-1.254199000
C	-3.918464000	-1.424636000	-2.495999000
C	-1.426850000	-3.921627000	-1.254199000
C	-0.725461000	-4.105808000	-2.495999000
C	2.682803000	-3.196502000	-1.254199000
C	3.193003000	-2.681171000	-2.495999000
C	4.109654000	0.725125000	-1.254199000
C	3.918464000	1.424636000	-2.495999000
C	1.426850000	3.921627000	-1.254199000
C	0.725461000	4.105808000	-2.495999000
C	-3.918464000	1.424636000	-2.495999000
C	-4.087972000	0.715299000	-3.748526000
C	-3.193003000	-2.681171000	-2.495999000
C	-2.663453000	-3.182638000	-3.748526000
C	0.725461000	-4.105808000	-2.495999000
C	1.424519000	-3.897937000	-3.748526000
C	3.918464000	-1.424636000	-2.495999000
C	4.087972000	-0.715299000	-3.748526000
C	3.193003000	2.681171000	-2.495999000
C	2.663453000	3.182638000	-3.748526000
C	-0.725461000	4.105808000	-2.495999000
C	-1.424519000	3.897937000	-3.748526000
C	-4.087972000	-0.715299000	-3.748526000
C	-3.912513000	-1.420640000	-5.010824000
C	-1.424519000	-3.897937000	-3.748526000
C	-0.725946000	-4.098656000	-5.010824000
C	2.663453000	-3.182638000	-3.748526000
C	3.186567000	-2.678015000	-5.010824000
C	4.087972000	0.715299000	-3.748526000
C	3.912513000	1.420640000	-5.010824000
C	1.424519000	3.897937000	-3.748526000
C	0.725946000	4.098656000	-5.010824000
C	-2.663453000	3.182638000	-3.748526000
C	-3.186567000	2.678015000	-5.010824000
C	-3.186567000	-2.678015000	-5.010824000
C	-2.712612000	-3.225744000	-6.250344000
C	0.725946000	-4.098656000	-5.010824000
C	1.437270000	-3.962063000	-6.250344000
C	3.912513000	-1.420640000	-5.010824000
C	4.149882000	-0.736319000	-6.250344000
C	3.186567000	2.678015000	-5.010824000
C	2.712612000	3.225744000	-6.250344000
C	-0.725946000	4.098656000	-5.010824000
C	-1.437270000	3.962063000	-6.250344000
C	-3.912513000	1.420640000	-5.010824000
C	-4.149882000	0.736319000	-6.250344000
C	-1.437270000	-3.962063000	-6.250344000

C	-0.692555000	-4.213496000	-7.464549000
C	2.712612000	-3.225744000	-6.250344000
C	3.302717000	-2.706518000	-7.464549000
C	4.149882000	0.736319000	-6.250344000
C	3.995272000	1.506978000	-7.464549000
C	1.437270000	3.962063000	-6.250344000
C	0.692555000	4.213496000	-7.464549000
C	-2.712612000	3.225744000	-6.250344000
C	-3.302717000	2.706518000	-7.464549000
C	-4.149882000	-0.736319000	-6.250344000
C	-3.995272000	-1.506978000	-7.464549000
C	0.692555000	-4.213496000	-7.464549000
H	1.226575000	-4.273198000	-8.421337000
C	3.995272000	-1.506978000	-7.464549000
H	4.313986000	-1.074354000	-8.421337000
C	3.302717000	2.706518000	-7.464549000
H	3.087411000	3.198844000	-8.421337000
C	-0.692555000	4.213496000	-7.464549000
H	-1.226575000	4.273198000	-8.421337000
C	-3.995272000	1.506978000	-7.464549000
H	-4.313986000	1.074354000	-8.421337000
C	-3.302717000	-2.706518000	-7.464549000
H	-3.087411000	-3.198844000	-8.421337000
H	1.226575000	-4.273198000	8.421337000
H	4.313986000	-1.074354000	8.421337000
H	3.087411000	3.198844000	8.421337000
H	-1.226575000	4.273198000	8.421337000
H	-4.313986000	1.074354000	8.421337000
H	-3.087411000	-3.198844000	8.421337000
H	-1.226575000	-4.273198000	-8.421337000
H	3.087411000	-3.198844000	-8.421337000
H	4.313986000	1.074354000	-8.421337000
H	1.226575000	4.273198000	-8.421337000
H	-3.087411000	3.198844000	-8.421337000
H	-4.313986000	-1.074354000	-8.421337000

Nanotube (6,6) u07v0s
B3LYP/STO-3G Energy: -6338.767157

H	3.885005000	-2.145307000	-9.055628000
C	3.457897000	-2.476825000	-8.100488000
H	0.069815000	-4.444823000	-9.054973000
C	-0.429979000	-4.240750000	-8.099323000
H	-3.837028000	-2.304119000	-9.050456000
C	-3.902273000	-1.765366000	-8.096370000
H	-3.885005000	2.145307000	-9.055628000
C	-3.457897000	2.476825000	-8.100488000
H	-0.069815000	4.444823000	-9.054973000
C	0.429979000	4.240750000	-8.099323000
H	3.837028000	2.304119000	-9.050456000
C	3.902273000	1.765366000	-8.096370000
C	2.479431000	-3.451278000	-8.101061000
C	1.772101000	-3.800914000	-6.882450000
C	-1.765658000	-3.890650000	-8.097917000
C	-2.421716000	-3.452943000	-6.878426000
C	-4.255060000	-0.430486000	-8.097275000
C	-4.194685000	0.359029000	-6.879744000
C	-2.479431000	3.451278000	-8.101061000
C	-1.772101000	3.800914000	-6.882450000
C	1.765658000	3.890650000	-8.097917000
C	2.421716000	3.452943000	-6.878426000
C	4.255060000	0.430486000	-8.097275000
C	4.194685000	-0.359029000	-6.879744000
C	0.358996000	-4.183357000	-6.881680000
C	-0.363622000	-4.142360000	-5.639967000
C	-3.459317000	-2.419968000	-6.877745000
C	-3.779776000	-1.768781000	-5.637266000
C	-3.809014000	1.771302000	-6.881160000

C	-3.407077000	2.376257000	-5.640910000
C	-0.358996000	4.183357000	-6.881680000
C	0.363622000	4.142360000	-5.639967000
C	3.459317000	2.419968000	-6.877745000
C	3.779776000	1.768781000	-5.637266000
C	3.809014000	-1.771302000	-6.881160000
C	3.407077000	-2.376257000	-5.640910000
C	-1.769164000	-3.772769000	-5.638446000
C	-2.389836000	-3.397533000	-4.378632000
C	-4.151636000	-0.363655000	-5.638196000
C	-4.132609000	0.363469000	-4.379734000
C	-2.377807000	3.402133000	-5.641507000
C	-1.742736000	3.753980000	-4.382220000
C	1.769164000	3.772769000	-5.638446000
C	2.389836000	3.397533000	-4.378632000
C	4.151636000	0.363655000	-5.638196000
C	4.132609000	-0.363469000	-4.379734000
C	2.377807000	-3.402133000	-5.641507000
C	1.742736000	-3.753980000	-4.382220000
C	-3.401414000	-2.388738000	-4.378060000
C	-3.777794000	-1.760494000	-3.120960000
C	-3.758999000	1.742223000	-4.381078000
C	-3.405490000	2.384443000	-3.124584000
C	-0.363458000	4.125597000	-4.381460000
C	0.367241000	4.143240000	-3.123556000
C	3.401414000	2.388738000	-4.378060000
C	3.777794000	1.760494000	-3.120960000
C	3.758999000	-1.742223000	-4.381078000
C	3.405490000	-2.384443000	-3.124584000
C	0.363458000	-4.125597000	-4.381460000
C	-0.367241000	-4.143240000	-3.123556000
C	-4.148367000	-0.367352000	-3.121831000
C	-4.156777000	0.360681000	-1.877516000
C	-2.385387000	3.402898000	-3.125171000
C	-1.762506000	3.777654000	-1.880048000
C	1.760556000	3.773748000	-3.122108000
C	2.394707000	3.420072000	-1.876451000
C	4.148367000	0.367352000	-3.121831000
C	4.156777000	-0.360681000	-1.877516000
C	2.385387000	-3.402898000	-3.125171000
C	1.762506000	-3.777654000	-1.880048000
C	-1.760556000	-3.773748000	-3.122108000
C	-2.394707000	-3.420072000	-1.876451000
C	-3.779633000	1.762177000	-1.878918000
C	-3.408837000	2.391517000	-0.630209000
C	-0.360746000	4.153724000	-1.879231000
C	0.367588000	4.147432000	-0.629160000
C	3.421794000	2.394401000	-1.875880000
C	3.777416000	1.757106000	-0.626629000
C	3.779633000	-1.762177000	-1.878918000
C	3.408837000	-2.391517000	-0.630209000
C	0.360746000	-4.153724000	-1.879231000
C	-0.367588000	-4.147432000	-0.629160000
C	-3.421794000	-2.394401000	-1.875880000
C	-3.777416000	-1.757106000	-0.626629000
C	-2.391815000	3.408352000	-0.630776000
C	-1.757086000	3.777385000	0.626627000
C	1.756972000	3.776426000	-0.627757000
C	2.391542000	3.408862000	0.630209000
C	4.148505000	0.367704000	-0.627459000
C	4.147436000	-0.367566000	0.629160000
C	2.391815000	-3.408352000	-0.630776000
C	1.757086000	-3.777385000	0.626627000
C	-1.756972000	-3.776426000	-0.627757000
C	-2.391542000	-3.408862000	0.630209000
C	-4.148505000	-0.367704000	-0.627459000
C	-4.147436000	0.367566000	0.629160000
C	-0.367690000	4.148490000	0.627458000
C	0.360688000	4.156776000	1.877518000
C	3.408381000	2.391843000	0.630774000

C	3.777676000	1.762539000	1.880050000
C	3.776410000	-1.756945000	0.627756000
C	3.420056000	-2.394671000	1.876452000
C	0.367690000	-4.148490000	0.627458000
C	-0.360688000	-4.156776000	1.877518000
C	-3.408381000	-2.391843000	0.630774000
C	-3.777676000	-1.762539000	1.880050000
C	-3.776410000	1.756945000	0.627756000
C	-3.420056000	2.394671000	1.876452000
C	1.762190000	3.779654000	1.878916000
C	2.384452000	3.405521000	3.124587000
C	4.153736000	0.360775000	1.879232000
C	4.143242000	-0.367207000	3.123558000
C	2.394385000	-3.421758000	1.875877000
C	1.760489000	-3.777762000	3.120959000
C	-1.762190000	-3.779654000	1.878916000
C	-2.384452000	-3.405521000	3.124587000
C	-4.153736000	-0.360775000	1.879232000
C	-4.143242000	0.367207000	3.123558000
C	-2.394385000	3.421758000	1.875877000
C	-1.760489000	3.777762000	3.120959000
C	3.402916000	2.385425000	3.125172000
C	3.753990000	1.742775000	4.382221000
C	3.773741000	-1.760518000	3.122106000
C	3.397529000	-2.389797000	4.378632000
C	0.367353000	-4.148357000	3.121829000
C	-0.363458000	-4.132606000	4.379738000
C	-3.402916000	-2.385425000	3.125172000
C	-3.753990000	-1.742775000	4.382221000
C	-3.773741000	1.760518000	3.122106000
C	-3.397529000	2.389797000	4.378632000
C	-0.367353000	4.148357000	3.121829000
C	0.363458000	4.132606000	4.379738000
C	4.125604000	0.363496000	4.381460000
C	4.142366000	-0.363583000	5.639967000
C	2.388740000	-3.401377000	4.378052000
C	1.768798000	-3.779743000	5.637265000
C	-1.742216000	-3.759019000	4.381079000
C	-2.376249000	-3.407102000	5.640914000
C	-4.125604000	-0.363496000	4.381460000
C	-4.142366000	0.363583000	5.639967000
C	-2.388740000	3.401377000	4.378052000
C	-1.768798000	3.779743000	5.637265000
C	1.742216000	3.759019000	4.381079000
C	2.376249000	3.407102000	5.640914000
C	3.772780000	-1.769125000	5.638444000
C	3.452966000	-2.421684000	6.878429000
C	0.363676000	-4.151622000	5.638196000
C	-0.358996000	-4.194677000	6.879751000
C	-3.402137000	-2.377845000	5.641511000
C	-3.800919000	-1.772142000	6.882454000
C	-3.772780000	1.769125000	5.638444000
C	-3.452966000	2.421684000	6.878429000
C	-0.363676000	4.151622000	5.638196000
C	0.358996000	4.194677000	6.879751000
C	3.402137000	2.377845000	5.641511000
C	3.800919000	1.772142000	6.882454000
C	2.419986000	-3.459278000	6.877735000
C	1.765397000	-3.902233000	8.096366000
C	-1.771280000	-3.809023000	6.881160000
C	-2.476791000	-3.457907000	8.100492000
C	-4.183368000	-0.359041000	6.881678000
C	-4.240785000	0.429949000	8.099317000
C	-2.419986000	3.459278000	6.877735000
C	-1.765397000	3.902233000	8.096366000
C	1.771280000	3.809023000	6.881160000
C	2.476791000	3.457907000	8.100492000
C	4.183368000	0.359041000	6.881678000
C	4.240785000	-0.429949000	8.099317000
C	0.430515000	-4.255033000	8.097278000

H	-0.068482000	-4.463980000	9.052317000
C	-3.451265000	-2.479458000	8.101068000
H	-3.876137000	-2.146692000	9.056785000
C	-3.890696000	1.765619000	8.097912000
H	-3.822930000	2.303845000	9.052144000
C	-0.430515000	4.255033000	8.097278000
H	0.068482000	4.463980000	9.052317000
C	3.451265000	2.479458000	8.101068000
H	3.876137000	2.146692000	9.056785000
C	3.890696000	-1.765619000	8.097912000
H	3.822930000	-2.303845000	9.052144000
H	2.146665000	-3.876164000	-9.056772000
H	-2.303859000	-3.822849000	-9.052155000
H	-4.464006000	0.068532000	-9.052304000
H	-2.146665000	3.876164000	-9.056772000
H	2.303859000	3.822849000	-9.052155000
H	4.464006000	-0.068532000	-9.052304000
H	2.304150000	-3.836954000	9.050447000
H	-2.145246000	-3.884992000	9.055631000
H	-4.444879000	-0.069870000	9.054953000
H	-2.304150000	3.836954000	9.050447000
H	2.145246000	3.884992000	9.055631000
H	4.444879000	0.069870000	9.054953000

Nanotube (6,6) u07v6s
B3LYP/STO-3G Energy: -6790.539231

C	-3.47371662	2.49069430	-8.70592662
C	-2.49069430	3.47371662	-8.70592662
C	0.42014623	4.25367399	-8.70592662
C	1.76297969	3.89386285	-8.70592662
C	3.89386285	1.76297969	-8.70592662
C	4.25367399	0.42014623	-8.70592662
C	3.47371662	-2.49069430	-8.70592662
C	2.49069430	-3.47371662	-8.70592662
C	-0.42014623	-4.25367399	-8.70592662
C	-1.76297969	-3.89386285	-8.70592662
C	-3.89386285	-1.76297969	-8.70592662
C	-4.25367399	-0.42014623	-8.70592662
C	-1.78982030	3.82239137	-7.49703426
C	-0.36116584	4.20519818	-7.49703426
C	2.41537788	3.46122553	-7.49703426
C	3.46122553	2.41537788	-7.49703426
C	4.20519818	-0.36116584	-7.49703426
C	3.82239137	-1.78982030	-7.49703426
C	1.78982030	-3.82239137	-7.49703426
C	0.36116584	-4.20519818	-7.49703426
C	-2.41537788	-3.46122553	-7.49703426
C	-3.46122553	-2.41537788	-7.49703426
C	-4.20519818	0.36116584	-7.49703426
C	-3.82239137	1.78982030	-7.49703426
C	0.36067017	4.14561205	-6.25672417
C	1.76045650	3.77054044	-6.25672417
C	3.77054044	1.76045650	-6.25672417
C	4.14561205	0.36067017	-6.25672417
C	3.40987027	-2.38515555	-6.25672417
C	2.38515555	-3.40987027	-6.25672417
C	-0.36067017	-4.14561205	-6.25672417
C	-1.76045650	-3.77054044	-6.25672417
C	-3.77054044	-1.76045650	-6.25672417
C	-4.14561205	-0.36067017	-6.25672417
C	-3.40987027	2.38515555	-6.25672417
C	-2.38515555	3.40987027	-6.25672417
C	2.38602000	3.40150377	-4.99232656
C	3.40150377	2.38602000	-4.99232656
C	4.13879868	-0.36560205	-4.99232656
C	3.76710582	-1.75277868	-4.99232656
C	1.75277868	-3.76710582	-4.99232656

C	0.36560205	-4.13879868	-4.99232656
C	-2.38602000	-3.40150377	-4.99232656
C	-3.40150377	-2.38602000	-4.99232656
C	-4.13879868	0.36560205	-4.99232656
C	-3.76710582	1.75277868	-4.99232656
C	-1.75277868	3.76710582	-4.99232656
C	-0.36560205	4.13879868	-4.99232656
C	3.78192672	1.76764661	-3.74631164
C	4.15906791	0.36013649	-3.74631164
C	3.42179022	-2.39142131	-3.74631164
C	2.39142131	-3.42179022	-3.74631164
C	-0.36013649	-4.15906791	-3.74631164
C	-1.76764661	-3.78192672	-3.74631164
C	-3.78192672	-1.76764661	-3.74631164
C	-4.15906791	-0.36013649	-3.74631164
C	-3.42179022	2.39142131	-3.74631164
C	-2.39142131	3.42179022	-3.74631164
C	0.36013649	4.15906791	-3.74631164
C	1.76764661	3.78192672	-3.74631164
C	4.15532033	-0.36497299	-2.50262476
C	3.78109946	-1.76158428	-2.50262476
C	1.76158428	-3.78109946	-2.50262476
C	0.36497299	-4.15532033	-2.50262476
C	-2.39373605	-3.41612647	-2.50262476
C	-3.41612647	-2.39373605	-2.50262476
C	-4.15532033	0.36497299	-2.50262476
C	-3.78109946	1.76158428	-2.50262476
C	-1.76158428	3.78109946	-2.50262476
C	-0.36497299	4.15532033	-2.50262476
C	2.39373605	3.41612647	-2.50262476
C	3.41612647	2.39373605	-2.50262476
C	3.41621738	-2.39486823	-1.24530563
C	2.39486823	-3.41621738	-1.24530563
C	-0.36590804	-4.15596515	-1.24530563
C	-1.76109692	-3.78212541	-1.24530563
C	-3.78212541	-1.76109692	-1.24530563
C	-4.15596515	-0.36590804	-1.24530563
C	-3.41621738	2.39486823	-1.24530563
C	-2.39486823	3.41621738	-1.24530563
C	0.36590804	4.15596515	-1.24530563
C	1.76109692	3.78212541	-1.24530563
C	3.78212541	1.76109692	-1.24530563
C	4.15596515	0.36590804	-1.24530563
C	1.76981361	-3.78842655	0.00000000
C	0.36150972	-4.16578044	0.00000000
C	-2.39596682	-3.42691682	0.00000000
C	-3.42691682	-2.39596682	0.00000000
C	-4.16578044	0.36150972	0.00000000
C	-3.78842655	1.76981361	0.00000000
C	-1.76981361	3.78842655	0.00000000
C	-0.36150972	4.16578044	0.00000000
C	2.39596682	3.42691682	0.00000000
C	3.42691682	2.39596682	0.00000000
C	4.16578044	-0.36150972	0.00000000
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C	-0.36590804	-4.15596515	1.24530563
C	-1.76109692	-3.78212541	1.24530563
C	-3.78212541	-1.76109692	1.24530563
C	-4.15596515	-0.36590804	1.24530563
C	-3.41621738	2.39486823	1.24530563
C	-2.39486823	3.41621738	1.24530563
C	0.36590804	4.15596515	1.24530563
C	1.76109692	3.78212541	1.24530563
C	3.78212541	1.76109692	1.24530563
C	4.15596515	0.36590804	1.24530563
C	3.41621738	-2.39486823	1.24530563
C	2.39486823	-3.41621738	1.24530563
C	-2.39373605	-3.41612647	2.50262476
C	-3.41612647	-2.39373605	2.50262476
C	-4.15532033	0.36497299	2.50262476

C	-3.78109946	1.76158428	2.50262476
C	-1.76158428	3.78109946	2.50262476
C	-0.36497299	4.15532033	2.50262476
C	2.39373605	3.41612647	2.50262476
C	3.41612647	2.39373605	2.50262476
C	4.15532033	-0.36497299	2.50262476
C	3.78109946	-1.76158428	2.50262476
C	1.76158428	-3.78109946	2.50262476
C	0.36497299	-4.15532033	2.50262476
C	-3.78192672	-1.76764661	3.74631164
C	-4.15906791	-0.36013649	3.74631164
C	-3.42179022	2.39142131	3.74631164
C	-2.39142131	3.42179022	3.74631164
C	0.36013649	4.15906791	3.74631164
C	1.76764661	3.78192672	3.74631164
C	3.78192672	1.76764661	3.74631164
C	4.15906791	0.36013649	3.74631164
C	3.42179022	-2.39142131	3.74631164
C	2.39142131	-3.42179022	3.74631164
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C	-1.76764661	-3.78192672	3.74631164
C	-4.13879868	0.36560205	4.99232656
C	-3.76710582	1.75277868	4.99232656
C	-1.75277868	3.76710582	4.99232656
C	-0.36560205	4.13879868	4.99232656
C	2.38602000	3.40150377	4.99232656
C	3.40150377	2.38602000	4.99232656
C	4.13879868	-0.36560205	4.99232656
C	3.76710582	-1.75277868	4.99232656
C	1.75277868	-3.76710582	4.99232656
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C	-2.38602000	-3.40150377	4.99232656
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C	-3.40987027	2.38515555	6.25672417
C	-2.38515555	3.40987027	6.25672417
C	0.36067017	4.14561205	6.25672417
C	1.76045650	3.77054044	6.25672417
C	3.77054044	1.76045650	6.25672417
C	4.14561205	0.36067017	6.25672417
C	3.40987027	-2.38515555	6.25672417
C	2.38515555	-3.40987027	6.25672417
C	-0.36067017	-4.14561205	6.25672417
C	-1.76045650	-3.77054044	6.25672417
C	-3.77054044	-1.76045650	6.25672417
C	-4.14561205	-0.36067017	6.25672417
C	-1.78982030	3.82239137	7.49703426
C	-0.36116584	4.20519818	7.49703426
C	2.41537788	3.46122553	7.49703426
C	3.46122553	2.41537788	7.49703426
C	4.20519818	-0.36116584	7.49703426
C	3.82239137	-1.78982030	7.49703426
C	1.78982030	-3.82239137	7.49703426
C	0.36116584	-4.20519818	7.49703426
C	-2.41537788	-3.46122553	7.49703426
C	-3.46122553	-2.41537788	7.49703426
C	-4.20519818	0.36116584	7.49703426
C	-3.82239137	1.78982030	7.49703426
C	0.42014623	4.25367399	8.70592662
C	1.76297969	3.89386285	8.70592662
C	3.89386285	1.76297969	8.70592662
C	4.25367399	0.42014623	8.70592662
C	3.47371662	-2.49069430	8.70592662
C	2.49069430	-3.47371662	8.70592662
C	-0.42014623	-4.25367399	8.70592662
C	-1.76297969	-3.89386285	8.70592662
C	-3.89386285	-1.76297969	8.70592662
C	-4.25367399	-0.42014623	8.70592662
C	-3.47371662	2.49069430	8.70592662
C	-2.49069430	3.47371662	8.70592662
H	-3.88542343	2.15162843	-9.66515970

H	-2.15162843	3.88542343	-9.66515970
H	-0.07934684	4.44068960	-9.66515970
H	2.28906118	3.80607659	-9.66515970
H	3.80607659	2.28906118	-9.66515970
H	4.44068960	-0.07934684	-9.66515970
H	3.88542343	-2.15162843	-9.66515970
H	2.15162843	-3.88542343	-9.66515970
H	0.07934684	-4.44068960	-9.66515970
H	-2.28906118	-3.80607659	-9.66515970
H	-3.80607659	-2.28906118	-9.66515970
H	-4.44068960	0.07934684	-9.66515970
H	-0.07934684	4.44068960	9.66515970
H	2.28906118	3.80607659	9.66515970
H	3.80607659	2.28906118	9.66515970
H	4.44068960	-0.07934684	9.66515970
H	3.88542343	-2.15162843	9.66515970
H	2.15162843	-3.88542343	9.66515970
H	0.07934684	-4.44068960	9.66515970
H	-2.28906118	-3.80607659	9.66515970
H	-3.80607659	-2.28906118	9.66515970
H	-4.44068960	0.07934684	9.66515970
H	-3.88542343	2.15162843	9.66515970
H	-2.15162843	3.88542343	9.66515970

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B3LYP/STO-3G Energy: -7242.327223

H	-3.198889	-3.087359	10.296727
C	-2.706573	-3.302436	9.339583
H	1.074286	-4.313999	10.296727
C	1.506707	-3.995179	9.339583
H	4.273176	-1.226640	10.296727
C	4.213280	-0.692743	9.339583
H	3.198889	3.087359	10.296727
C	2.706573	3.302436	9.339583
H	-1.074286	4.313999	10.296727
C	-1.506707	3.995179	9.339583
H	-4.273176	1.226640	10.296727
C	-4.213280	0.692743	9.339583
C	-1.506707	-3.995179	9.339583
C	-0.736316	-4.149843	8.125684
C	2.706573	-3.302436	9.339583
C	3.225712	-2.712590	8.125684
C	4.213280	0.692743	9.339583
C	3.962028	1.437253	8.125684
C	1.506707	3.995179	9.339583
C	0.736316	4.149843	8.125684
C	-2.706573	3.302436	9.339583
C	-3.225712	2.712590	8.125684
C	-4.213280	-0.692743	9.339583
C	-3.962028	-1.437253	8.125684
C	0.736316	-4.149843	8.125684
C	1.420496	-3.911818	6.885921
C	3.962028	-1.437253	8.125684
C	4.097982	-0.725723	6.885921
C	3.225712	2.712590	8.125684
C	2.677486	3.186095	6.885921
C	-0.736316	4.149843	8.125684
C	-1.420496	3.911818	6.885921
C	-3.962028	1.437253	8.125684
C	-4.097982	0.725723	6.885921
C	-3.225712	-2.712590	8.125684
C	-2.677486	-3.186095	6.885921
C	2.677486	-3.186095	6.885921
C	3.182574	-2.663726	5.623387
C	4.097982	0.725723	6.885921
C	3.898141	1.424327	5.623387
C	1.420496	3.911818	6.885921

C	0.715567	4.088053	5.623387
C	-2.677486	3.186095	6.885921
C	-3.182574	2.663726	5.623387
C	-4.097982	-0.725723	6.885921
C	-3.898141	-1.424327	5.623387
C	-1.420496	-3.911818	6.885921
C	-0.715567	-4.088053	5.623387
C	3.898141	-1.424327	5.623387
C	4.105692	-0.725524	4.371435
C	3.182574	2.663726	5.623387
C	2.681168	3.192871	4.371435
C	-0.715567	4.088053	5.623387
C	-1.424524	3.918395	4.371435
C	-3.898141	1.424327	5.623387
C	-4.105692	0.725524	4.371435
C	-3.182574	-2.663726	5.623387
C	-2.681168	-3.192871	4.371435
C	0.715567	-4.088053	5.623387
C	1.424524	-3.918395	4.371435
C	4.105692	0.725524	4.371435
C	3.920346	1.426645	3.129086
C	1.424524	3.918395	4.371435
C	0.724662	4.108442	3.129086
C	-2.681168	3.192871	4.371435
C	-3.195684	2.681796	3.129086
C	-4.105692	-0.725524	4.371435
C	-3.920346	-1.426645	3.129086
C	-1.424524	-3.918395	4.371435
C	-0.724662	-4.108442	3.129086
C	2.681168	-3.192871	4.371435
C	3.195684	-2.681796	3.129086
C	3.195684	2.681796	3.129086
C	2.674301	3.194041	1.874515
C	-0.724662	4.108442	3.129086
C	-1.428970	3.913033	1.874515
C	-3.920346	1.426645	3.129086
C	-4.103271	0.718993	1.874515
C	-3.195684	-2.681796	3.129086
C	-2.674301	-3.194041	1.874515
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C	3.920346	-1.426645	3.129086
C	4.103271	-0.718993	1.874515
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C	-2.674301	3.194041	1.874515
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Nanotube (6,6) u08v6_
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H	2.292656510	3.814861350	-10.928718630
H	3.814861350	2.292656510	-10.928718630
H	4.450095100	-0.078068100	-10.928718630
H	3.892929460	-2.157438590	-10.928718630
H	2.157438590	-3.892929460	-10.928718630
H	0.078068100	-4.450095100	-10.928718630
H	-2.292656510	-3.814861350	-10.928718630
H	-3.814861350	-2.292656510	-10.928718630
H	-4.450095100	0.078068100	-10.928718630
H	3.814861350	2.292656510	10.928718630
H	4.450095100	-0.078068100	10.928718630
H	3.892929460	-2.157438590	10.928718630
H	2.157438590	-3.892929460	10.928718630
H	0.078068100	-4.450095100	10.928718630
H	-2.292656510	-3.814861350	10.928718630
H	-3.814861350	-2.292656510	10.928718630
H	-4.450095100	0.078068100	10.928718630
H	-3.892929460	2.157438590	10.928718630
H	-2.157438590	3.892929460	10.928718630
H	-0.078068100	4.450095100	10.928718630
H	2.292656510	3.814861350	10.928718630

Nanotube (6,6) u09v0s
B3LYP/STO-3G Energy: -8145.863334

C	-3.98682969	1.50593510	-10.60884018
C	-3.29759103	2.69972495	-10.60880804
C	-0.68923679	4.20566334	-10.60884018
C	0.68923488	4.20566007	-10.60880804
C	3.29759289	2.69972824	-10.60884018

C	3.98682590	1.50593512	-10.60880804
C	3.98682969	-1.50593510	-10.60884018
C	3.29759103	-2.69972495	-10.60880804
C	0.68923679	-4.20566334	-10.60884018
C	-0.68923488	-4.20566007	-10.60880804
C	-3.29759289	-2.69972824	-10.60884018
C	-3.98682590	-1.50593512	-10.60880804
C	-2.70052119	3.21815947	-9.38720040
C	-1.43674286	3.94779832	-9.38715724
C	1.43674726	3.94779969	-9.38720040
C	2.70052221	3.21815498	-9.38715724
C	4.13726845	0.72964022	-9.38720040
C	4.13726507	-0.72964334	-9.38715724
C	2.70052119	-3.21815947	-9.38720040
C	1.43674286	-3.94779832	-9.38715724
C	-1.43674726	-3.94779969	-9.38720040
C	-2.70052221	-3.21815498	-9.38715724
C	-4.13726845	-0.72964022	-9.38720040
C	-4.13726507	0.72964334	-9.38715724
C	-0.72667323	4.09687011	-8.14471227
C	0.72667106	4.09686910	-8.14466806
C	3.18465697	2.67775254	-8.14471227
C	3.91132824	1.41911895	-8.14466806
C	3.91133021	-1.41911757	-8.14471227
C	3.18465718	-2.67775014	-8.14466806
C	0.72667323	-4.09687011	-8.14471227
C	-0.72667106	-4.09686910	-8.14466806
C	-3.18465697	-2.67775254	-8.14471227
C	-3.91132824	-1.41911895	-8.14466806
C	-3.91133021	1.41911757	-8.14471227
C	-3.18465718	2.67775014	-8.14466806
C	1.42323831	3.89374612	-6.88704852
C	2.66046454	3.17943434	-6.88701585
C	4.08370221	0.71431253	-6.88704852
C	4.08370318	-0.71431271	-6.88701585
C	2.66046390	-3.17943359	-6.88704852
C	1.42323864	-3.89374705	-6.88701585
C	-1.42323831	-3.89374612	-6.88704852
C	-2.66046454	-3.17943434	-6.88701585
C	-4.08370221	-0.71431253	-6.88704852
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C	-2.66046390	3.17943359	-6.88704852
C	-1.42323864	3.89374705	-6.88701585
C	3.18688049	2.66956827	-5.62833658
C	3.90535501	1.42513506	-5.62831599
C	3.90535418	-1.42513533	-5.62833658
C	3.18688067	-2.66956912	-5.62831599
C	0.71847369	-4.09470360	-5.62833658
C	-0.71847434	-4.09470418	-5.62831599
C	-3.18688049	-2.66956827	-5.62833658
C	-3.90535501	-1.42513506	-5.62831599
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C	-3.18688067	2.66956912	-5.62831599
C	-0.71847369	4.09470360	-5.62833658
C	0.71847434	4.09470418	-5.62831599
C	4.10702878	0.72484548	-4.38033141
C	4.10702928	-0.72484550	-4.38032238
C	2.68124900	-3.19436852	-4.38033141
C	1.42578002	-3.91921444	-4.38032238
C	-1.42577979	-3.91921400	-4.38033141
C	-2.68124926	-3.19436894	-4.38032238
C	-4.10702878	-0.72484548	-4.38033141
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C	-1.42578002	3.91921444	-4.38032238
C	1.42577979	3.91921400	-4.38033141
C	2.68124926	3.19436894	-4.38032238
C	3.91419490	-1.42818149	-3.13248883
C	3.19394162	-2.67570107	-3.13249314
C	0.72025600	-4.10388297	-3.13248883

C	-0.72025429	-4.10388511	-3.13249314
C	-3.19393890	-2.67570148	-3.13248883
C	-3.91419591	-1.42818404	-3.13249314
C	-3.91419490	1.42818149	-3.13248883
C	-3.19394162	2.67570107	-3.13249314
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C	0.72025429	4.10388511	-3.13249314
C	3.19393890	2.67570148	-3.13248883
C	3.91419591	1.42818404	-3.13249314
C	2.67169739	-3.19228711	-1.87627516
C	1.42875416	-3.90990181	-1.87629126
C	-1.42875304	-3.90990136	-1.87627516
C	-2.67169721	-3.19228830	-1.87629126
C	-4.10045043	-0.71761425	-1.87627516
C	-4.10045137	0.71761351	-1.87629126
C	-2.67169739	3.19228711	-1.87627516
C	-1.42875416	3.90990181	-1.87629126
C	1.42875304	3.90990136	-1.87627516
C	2.67169721	3.19228830	-1.87629126
C	4.10045043	0.71761425	-1.87627516
C	4.10045137	-0.71761351	-1.87629126
C	0.72311236	-4.10563534	-0.62318499
C	-0.72311071	-4.10563540	-0.62321106
C	-3.19402833	-2.67905134	-0.62318499
C	-3.91713991	-1.42658545	-0.62321106
C	-3.91714068	1.42658400	-0.62318499
C	-3.19402920	2.67904995	-0.62321106
C	-0.72311236	4.10563534	-0.62318499
C	0.72311071	4.10563540	-0.62321106
C	3.19402833	2.67905134	-0.62318499
C	3.91713991	1.42658545	-0.62321106
C	3.91714068	-1.42658400	-0.62318499
C	3.19402920	-2.67904995	-0.62321106
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C	-2.67905134	-3.19402833	0.62318499
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C	-4.10563534	0.72311236	0.62318499
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C	-1.42658400	3.91714068	0.62318499
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C	4.10563540	0.72311071	0.62321106
C	4.10563534	-0.72311236	0.62318499
C	2.67904995	-3.19402920	0.62321106
C	1.42658400	-3.91714068	0.62318499
C	-3.19228830	-2.67169721	1.87629126
C	-3.90990136	-1.42875304	1.87627516
C	-3.90990181	1.42875416	1.87629126
C	-3.19228711	2.67169739	1.87627516
C	-0.71761351	4.10045137	1.87629126
C	0.71761425	4.10045043	1.87627516
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C	3.90990136	1.42875304	1.87627516
C	3.90990181	-1.42875416	1.87629126
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C	-2.67570107	3.19394162	3.13249314
C	-1.42818149	3.91419490	3.13248883
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C	2.67570148	3.19393890	3.13248883
C	4.10388511	0.72025429	3.13249314
C	4.10388297	-0.72025600	3.13248883
C	2.67570107	-3.19394162	3.13249314
C	1.42818149	-3.91419490	3.13248883
C	-1.42818404	-3.91419591	3.13249314
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C	-3.91921444	1.42578002	4.38032238

C	-3.19436852	2.68124900	4.38033141
C	-0.72484550	4.10702928	4.38032238
C	0.72484548	4.10702878	4.38033141
C	3.19436894	2.68124926	4.38032238
C	3.91921400	1.42577979	4.38033141
C	3.91921444	-1.42578002	4.38032238
C	3.19436852	-2.68124900	4.38033141
C	0.72484550	-4.10702928	4.38032238
C	-0.72484548	-4.10702878	4.38033141
C	-3.19436894	-2.68124926	4.38032238
C	-3.91921400	-1.42577979	4.38033141
C	-2.66956912	3.18688067	5.62831599
C	-1.42513533	3.90535418	5.62833658
C	1.42513506	3.90535501	5.62831599
C	2.66956827	3.18688049	5.62833658
C	4.09470418	0.71847434	5.62831599
C	4.09470360	-0.71847369	5.62833658
C	2.66956912	-3.18688067	5.62831599
C	1.42513533	-3.90535418	5.62833658
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C	-0.71431271	4.08370318	6.88701585
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C	3.17943434	2.66046454	6.88701585
C	3.89374612	1.42323831	6.88704852
C	3.89374705	-1.42323864	6.88701585
C	3.17943359	-2.66046390	6.88704852
C	0.71431271	-4.08370318	6.88701585
C	-0.71431253	-4.08370221	6.88704852
C	-3.17943434	-2.66046454	6.88701585
C	-3.89374612	-1.42323831	6.88704852
C	-3.89374705	1.42323864	6.88701585
C	-3.17943359	2.66046390	6.88704852
C	1.41911895	3.91132824	8.14466806
C	2.67775254	3.18465697	8.14471227
C	4.09686910	0.72667106	8.14466806
C	4.09687011	-0.72667323	8.14471227
C	2.67775014	-3.18465718	8.14466806
C	1.41911757	-3.91133021	8.14471227
C	-1.41911895	-3.91132824	8.14466806
C	-2.67775254	-3.18465697	8.14471227
C	-4.09686910	-0.72667106	8.14466806
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C	-2.67775014	3.18465718	8.14466806
C	-1.41911757	3.91133021	8.14471227
C	3.21815498	2.70052221	9.38715724
C	3.94779969	1.43674726	9.38720040
C	3.94779832	-1.43674286	9.38715724
C	3.21815947	-2.70052119	9.38720040
C	0.72964334	-4.13726507	9.38715724
C	-0.72964022	-4.13726845	9.38720040
C	-3.21815498	-2.70052221	9.38715724
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C	-0.72964334	4.13726507	9.38715724
C	0.72964022	4.13726845	9.38720040
C	4.20566007	0.68923488	10.60880804
C	4.20566334	-0.68923679	10.60884018
C	2.69972495	-3.29759103	10.60880804
C	1.50593510	-3.98682969	10.60884018
C	-1.50593512	-3.98682590	10.60880804
C	-2.69972824	-3.29759289	10.60884018
C	-4.20566007	-0.68923488	10.60880804
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H	-4.32087383	1.07694119	-11.56235083
H	-3.09309698	3.20352313	-11.56236179
H	-1.22777848	4.28045710	-11.56235083
H	1.22778392	4.28046213	-11.56236179
H	3.09309534	3.20351590	-11.56235083
H	4.32088090	1.07693900	-11.56236179
H	4.32087383	-1.07694119	-11.56235083
H	3.09309698	-3.20352313	-11.56236179
H	1.22777848	-4.28045710	-11.56235083
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H	-4.32088090	-1.07693900	-11.56236179
H	4.28046213	1.22778392	11.56236179
H	4.28045710	-1.22777848	11.56235083
H	3.20352313	-3.09309698	11.56236179
H	1.07694119	-4.32087383	11.56235083
H	-1.07693900	-4.32088090	11.56236179
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H	-4.28046213	-1.22778392	11.56236179
H	-4.28045710	1.22777848	11.56235083
H	-3.20352313	3.09309698	11.56236179
H	-1.07694119	4.32087383	11.56235083
H	1.07693900	4.32088090	11.56236179
H	3.20351590	3.09309534	11.56235083

Nanotube (6,6) u09v6_
B3LYP/STO-3G Energy: -8597.657855

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C	-2.483172590	-3.462917060	11.218168120
C	0.419032020	-4.240560440	11.218168120
C	1.757387850	-3.881949080	11.218168120
C	3.881949080	-1.757387850	11.218168120
C	4.240560440	-0.419032020	11.218168120
C	3.462917060	2.483172590	11.218168120
C	2.483172590	3.462917060	11.218168120
C	-0.419032020	4.240560440	11.218168120
C	-1.757387850	3.881949080	11.218168120
C	-4.197556300	-0.362322490	10.002998330
C	-3.816351640	-1.784997670	10.002998330
C	-1.784997670	-3.816351640	10.002998330
C	-0.362322490	-4.197556300	10.002998330
C	2.412558630	-3.454029150	10.002998330
C	3.454029150	-2.412558630	10.002998330
C	4.197556300	0.362322490	10.002998330
C	3.816351640	1.784997670	10.002998330
C	1.784997670	3.816351640	10.002998330
C	0.362322490	4.197556300	10.002998330
C	-2.412558630	3.454029150	10.002998330
C	-3.454029150	2.412558630	10.002998330
C	-3.411124300	-2.384915380	8.762968080
C	-2.384915380	-3.411124300	8.762968080
C	0.359835150	-4.146577990	8.762968080
C	1.761662610	-3.770959450	8.762968080
C	3.770959450	-1.761662610	8.762968080
C	4.146577990	-0.359835150	8.762968080
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C	2.384915380	3.411124300	8.762968080
C	-0.359835150	4.146577990	8.762968080
C	-1.761662610	3.770959450	8.762968080
C	-3.770959450	1.761662610	8.762968080
C	-4.146577990	0.359835150	8.762968080
C	-1.749625630	-3.764309010	7.500163360
C	-0.366934260	-4.134800040	7.500163360
C	2.385174420	-3.397374740	7.500163360

C	3.397374740	-2.385174420	7.500163360
C	4.134800040	0.366934260	7.500163360
C	3.764309010	1.749625630	7.500163360
C	1.749625630	3.764309010	7.500163360
C	0.366934260	4.134800040	7.500163360
C	-2.385174420	3.397374740	7.500163360
C	-3.397374740	2.385174420	7.500163360
C	-4.134800040	-0.366934260	7.500163360
C	-3.764309010	-1.749625630	7.500163360
C	0.361687520	-4.153723770	6.248444090
C	1.763631310	-3.778074060	6.248444090
C	3.778074060	-1.763631310	6.248444090
C	4.153723770	-0.361687520	6.248444090
C	3.416386550	2.390092460	6.248444090
C	2.390092460	3.416386550	6.248444090
C	-0.361687520	4.153723770	6.248444090
C	-1.763631310	3.778074060	6.248444090
C	-3.778074060	1.763631310	6.248444090
C	-4.153723770	0.361687520	6.248444090
C	-3.416386550	-2.390092460	6.248444090
C	-2.390092460	-3.416386550	6.248444090
C	2.393068550	-3.417770040	5.005778600
C	3.417770040	-2.393068550	5.005778600
C	4.156409950	0.363573130	5.005778600
C	3.781343170	1.763341410	5.005778600
C	1.763341410	3.781343170	5.005778600
C	0.363573130	4.156409950	5.005778600
C	-2.393068550	3.417770040	5.005778600
C	-3.417770040	2.393068550	5.005778600
C	-4.156409950	-0.363573130	5.005778600
C	-3.781343170	-1.763341410	5.005778600
C	-1.763341410	-3.781343170	5.005778600
C	-0.363573130	-4.156409950	5.005778600
C	3.777142650	-1.756765750	3.750990760
C	4.149484360	-0.367167560	3.750990760
C	3.409975090	2.392718620	3.750990760
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C	-0.367167560	4.149484360	3.750990760
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C	1.756765750	-3.777142650	3.750990760
C	4.156985330	0.363033570	2.498247710
C	3.781571680	1.764096370	2.498247710
C	1.764096370	3.781571680	2.498247710
C	0.363033570	4.156985330	2.498247710
C	-2.392888960	3.418538120	2.498247710
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C	-1.764096370	-3.781571680	2.498247710
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C	3.418538120	-2.392888960	2.498247710
C	3.418063760	2.392973180	1.253850130
C	2.392973180	3.418063760	1.253850130
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C	-1.763643460	3.781407450	1.253850130
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C	1.764096370	3.781571680	-2.498247710
C	0.363033570	4.156985330	-2.498247710
C	-3.777142650	1.756765750	-3.750990760
C	-4.149484360	0.367167560	-3.750990760
C	-3.409975090	-2.392718620	-3.750990760
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C	1.756765750	-3.777142650	-3.750990760
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C	-1.756765750	3.777142650	-3.750990760
C	-4.156409950	-0.363573130	-5.005778600
C	-3.781343170	-1.763341410	-5.005778600
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C	2.393068550	-3.417770040	-5.005778600
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C	0.361687520	-4.153723770	-6.248444090
C	1.763631310	-3.778074060	-6.248444090
C	3.778074060	-1.763631310	-6.248444090
C	4.153723770	-0.361687520	-6.248444090
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C	-4.153723770	0.361687520	-6.248444090
C	-1.749625630	-3.764309010	-7.500163360
C	-0.366934260	-4.134800040	-7.500163360
C	2.385174420	-3.397374740	-7.500163360
C	3.397374740	-2.385174420	-7.500163360
C	4.134800040	0.366934260	-7.500163360
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C	1.761662610	-3.770959450	-8.762968080
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C	4.146577990	-0.359835150	-8.762968080
C	3.411124300	2.384915380	-8.762968080
C	2.384915380	3.411124300	-8.762968080
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C	-2.384915380	-3.411124300	-8.762968080
C	2.412558630	-3.454029150	-10.002998330
C	3.454029150	-2.412558630	-10.002998330
C	4.197556300	0.362322490	-10.002998330
C	3.816351640	1.784997670	-10.002998330
C	1.784997670	3.816351640	-10.002998330
C	0.362322490	4.197556300	-10.002998330
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C	-1.784997670	-3.816351640	-10.002998330
C	-0.362322490	-4.197556300	-10.002998330
C	3.881949080	-1.757387850	-11.218168120
C	4.240560440	-0.419032020	-11.218168120
C	3.462917060	2.483172590	-11.218168120
C	2.483172590	3.462917060	-11.218168120
C	-0.419032020	4.240560440	-11.218168120
C	-1.757387850	3.881949080	-11.218168120
C	-3.881949080	1.757387850	-11.218168120
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C	-2.483172590	-3.462917060	-11.218168120
C	0.419032020	-4.240560440	-11.218168120
C	1.757387850	-3.881949080	-11.218168120
H	-3.790597880	2.284652960	12.176339860
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H	-3.873866440	-2.140427580	12.176339860
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H	2.284652960	-3.790597880	12.176339860
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H	2.140427580	3.873866440	-12.176339860
H	0.083268560	4.425080540	-12.176339860
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H	-0.083268560	-4.425080540	-12.176339860
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Nanotube (6,6) u10v0s
B3LYP/STO-3G Energy: -9049.433271

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C	-3.295313710	2.700617550	-11.850753740
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C	2.707542680	3.222318430	-10.632613400
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C	4.144380960	-0.733641530	-10.632613400
C	2.707541060	-3.222319860	-10.632596750
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C	2.662375120	3.181791070	-8.131598290
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C	4.086699450	-0.714788950	-8.131598290
C	2.662374150	-3.181792210	-8.131594330
C	1.424324330	-3.896580020	-8.131598290
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C	3.913111020	-1.424804810	-6.876167390
C	3.190470750	-2.676452090	-6.876162410
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C	3.911581500	1.428391780	-4.380513970
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C	-2.676745990	-3.193253450	-3.124321740
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C	-0.725640920	-4.108827510	-1.877290200
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C	-3.921169460	-1.425990280	-1.877290200
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C	-4.102792000	0.720066150	-0.628253850
C	-2.674992640	3.193089450	-0.628239690
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C	1.427800260	3.913156310	-0.628239690
C	2.674991580	3.193089020	-0.628253850
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C	4.102792000	-0.720066150	-0.628253850
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C	-0.720066150	4.102792000	0.628253850
C	0.720066850	4.102792900	0.628239690
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Nanotube (6,6) u10v6s
B3LYP/STO-3G Energy: -9501.198813

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C	-4.144605970	-0.365391260	7.505706150
C	-3.406638420	2.388741100	7.505706150
C	-2.388741100	3.406638420	7.505706150
C	0.365391260	4.144605970	7.505706150
C	1.755864870	3.772029690	7.505706150
C	4.132044350	-0.367416970	8.763445860
C	3.762163860	-1.747829740	8.763445860
C	1.747829740	-3.762163860	8.763445860
C	0.367416970	-4.132044350	8.763445860
C	-2.384214600	-3.394746890	8.763445860
C	-3.394746890	-2.384214600	8.763445860
C	-4.132044350	0.367416970	8.763445860

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C	-1.747829740	3.762163860	8.763445860
C	-0.367416970	4.132044350	8.763445860
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C	3.394746890	2.384214600	8.763445860
C	3.413226750	-2.385148180	10.021618180
C	2.385148180	-3.413226750	10.021618180
C	-0.358985540	-4.148515170	10.021618180
C	-1.763366990	-3.772212290	10.021618180
C	-3.772212290	-1.763366990	10.021618180
C	-4.148515170	-0.358985540	10.021618180
C	-3.413226750	2.385148180	10.021618180
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C	0.358985540	4.148515170	10.021618180
C	1.763366990	3.772212290	10.021618180
C	3.772212290	1.763366990	10.021618180
C	4.148515170	0.358985540	10.021618180
C	1.777775150	-3.810445000	11.263137520
C	0.365624060	-4.188829750	11.263137520
C	-2.411054600	-3.444820940	11.263137520
C	-3.444820940	-2.411054600	11.263137520
C	-4.188829750	0.365624060	11.263137520
C	-3.810445000	1.777775150	11.263137520
C	-1.777775150	3.810445000	11.263137520
C	-0.365624060	4.188829750	11.263137520
C	2.411054600	3.444820940	11.263137520
C	3.444820940	2.411054600	11.263137520
C	4.188829750	-0.365624060	11.263137520
C	3.810445000	-1.777775150	11.263137520
C	-0.421942740	-4.239760630	12.483581840
C	-1.754467190	-3.882711780	12.483581840
C	-3.882711780	-1.754467190	12.483581840
C	-4.239760630	-0.421942740	12.483581840
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C	0.421942740	4.239760630	12.483581840
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C	3.882711780	1.754467190	12.483581840
C	4.239760630	0.421942740	12.483581840
C	3.460769040	-2.485293440	12.483581840
C	2.485293440	-3.460769040	12.483581840
H	-3.889324730	2.153095930	-13.437912180
H	-2.153095930	3.889324730	-13.437912180
H	-0.080026600	4.444801980	-13.437912180
H	2.291706060	3.809298140	-13.437912180
H	3.809298140	2.291706060	-13.437912180
H	4.444801980	-0.080026600	-13.437912180
H	3.889324730	-2.153095930	-13.437912180
H	2.153095930	-3.889324730	-13.437912180
H	0.080026600	-4.444801980	-13.437912180
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H	-4.444801980	0.080026600	-13.437912180
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H	-2.291706060	-3.809298140	13.437912180
H	-3.809298140	-2.291706060	13.437912180
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Nanotube (6,6) ullv0s
B3LYP/STO-3G Energy: -9952.988914

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C	0.693007630	4.212644320	-13.089550710
C	3.301739120	2.706474830	-13.089378510
C	3.994760810	1.506159950	-13.089550710
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C	-3.301739120	-2.706474830	-13.089378510
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C	-1.437340210	3.962951020	-11.875849300
C	1.437335750	3.962942470	-11.875659710
C	2.713346150	3.226248650	-11.875849300
C	4.150676730	0.736701960	-11.875659710
C	4.150686360	-0.736702370	-11.875849300
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C	-4.150686360	0.736702370	-11.875849300
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C	3.913654320	-1.421421170	-10.635903940
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C	2.665062120	3.183869150	-9.373512280
C	4.089843650	0.716072710	-9.373462790
C	4.089842630	-0.716076920	-9.373512280
C	2.665058980	-3.183872140	-9.373462790
C	1.424780510	-3.899946080	-9.373512280
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C	3.194220810	2.682395530	-8.122130910
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C	3.920133080	-1.425078600	-8.122130910
C	3.194218100	-2.682398640	-8.122126280
C	0.725912260	-4.107474130	-8.122130910
C	-0.725916310	-4.107473340	-8.122126280
C	-3.194220810	-2.682395530	-8.122130910
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C	4.108706990	-0.724460910	-6.879487000
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C	1.426951940	-3.920475080	-6.879487000
C	-1.426950360	-3.920475650	-6.879516810
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C	1.426521610	-3.921520390	-4.372447810
C	-1.426519100	-3.921520720	-4.372473750
C	-2.682875480	-3.196164150	-4.372447810
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C	-4.103759970	0.719946280	-1.874991000
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C	-1.428388220	3.913933520	-1.874991000
C	1.428387640	3.913934730	-1.874994000
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C	-0.725356240	4.109397090	4.372447810
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C	3.921520720	1.426519100	4.372473750
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C	3.196162140	-2.682877020	4.372473750
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C	-3.196164150	-2.682875480	4.372447810
C	-3.921520720	-1.426519100	4.372473750
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C	-0.736702370	4.150686360	11.875849300
C	0.736701960	4.150676730	11.875659710
C	3.226248650	2.713346150	11.875849300
C	3.962942470	1.437335750	11.875659710
C	3.962951020	-1.437340210	11.875849300
C	3.226240510	-2.713340980	11.875659710
C	-1.506159950	-3.994760810	13.089550710
C	-2.706474830	-3.301739120	13.089378510
C	-4.212644320	-0.693007630	13.089550710
C	-4.212627370	0.693006390	13.089378510
C	-2.706484370	3.301753180	13.089550710
C	-1.506152540	3.994745520	13.089378510
C	1.506159950	3.994760810	13.089550710
C	2.706474830	3.301739120	13.089378510
C	4.212644320	0.693007630	13.089550710
C	4.212627370	-0.693006390	13.089378510
C	2.706484370	-3.301753180	13.089550710
C	1.506152540	-3.994745520	13.089378510
H	-4.311510340	1.072285220	-14.046632800
H	-3.084390650	3.197707200	-14.046574680
H	-1.227128940	4.270020090	-14.046632800
H	1.227100340	4.270014260	-14.046574680
H	3.084381410	3.197734880	-14.046632800
H	4.311490990	1.072307060	-14.046574680
H	4.311510340	-1.072285220	-14.046632800
H	3.084390650	-3.197707200	-14.046574680
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H	-4.311490990	-1.072307060	-14.046574680
H	-1.072307060	-4.311490990	14.046574680
H	-3.197734880	-3.084381410	14.046632800
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H	-4.270020090	1.227128940	14.046632800
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H	3.197734880	3.084381410	14.046632800
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H	4.270020090	-1.227128940	14.046632800
H	3.197707200	-3.084390650	14.046574680
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Nanotube (6,6) ullv6s
B3LYP/STO-3G Energy: -10404.765641

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C	-2.490652600	3.468746590	-13.721254670
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C	1.758696370	3.891341720	-13.721254670
C	3.891341720	1.758696370	-13.721254670
C	4.249348970	0.422595130	-13.721254670
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C	-1.758696370	-3.891341720	-13.721254670
C	-3.891341720	-1.758696370	-13.721254670
C	-4.249348970	-0.422595130	-13.721254670
C	-1.782696710	3.815927190	-12.505022250
C	-0.364102960	4.196038240	-12.505022250
C	2.413341530	3.451824230	-12.505022250
C	3.451824230	2.413341530	-12.505022250
C	4.196038240	-0.364102960	-12.505022250
C	3.815927190	-1.782696710	-12.505022250
C	1.782696710	-3.815927190	-12.505022250
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C	-2.413341530	-3.451824230	-12.505022250
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C	-4.196038240	0.364102960	-12.505022250
C	-3.815927190	1.782696710	-12.505022250
C	0.359408710	4.147892410	-11.264953400
C	1.762689140	3.771884560	-11.264953400
C	3.771884560	1.762689140	-11.264953400
C	4.147892410	0.359408710	-11.264953400
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C	-0.359408710	-4.147892410	-11.264953400
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C	-2.385203280	3.412475850	-11.264953400
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C	3.395702400	2.384509160	-10.004356640
C	4.133019120	-0.367194310	-10.004356640
C	3.762896710	-1.748509960	-10.004356640
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C	0.367194310	-4.133019120	-10.004356640
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C	-0.367194310	4.133019120	-10.004356640
C	3.775896960	1.760536190	-8.749928300
C	4.150290780	0.363279410	-8.749928300
C	3.412617540	-2.389754590	-8.749928300
C	2.389754590	-3.412617540	-8.749928300
C	-0.363279410	-4.150290780	-8.749928300
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C	-4.150290780	-0.363279410	-8.749928300
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C	-2.389754590	3.412617540	-8.749928300
C	0.363279410	4.150290780	-8.749928300
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C	4.156408240	-0.362876520	-7.506482580
C	3.780993390	-1.763943840	-7.506482580
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C	0.362876520	-4.156408240	-7.506482580
C	-2.392464410	-3.418116870	-7.506482580
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C	-0.367185990	-4.147721020	-6.254538330
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C	3.775624770	1.755868120	-6.254538330
C	4.147721020	0.367185990	-6.254538330
C	1.759912400	-3.778275600	-4.999049770
C	0.365008950	-4.152038850	-4.999049770
C	-2.392126450	-3.413266650	-4.999049770
C	-3.413266650	-2.392126450	-4.999049770
C	-4.152038850	0.365008950	-4.999049770
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C	-1.759912400	3.778275600	-4.999049770
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C	3.413266650	2.392126450	-4.999049770
C	4.152038850	-0.365008950	-4.999049770
C	3.778275600	-1.759912400	-4.999049770
C	-0.362903330	-4.156884560	-3.752957930
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C	2.392725790	-3.418515960	-3.752957930
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C	-1.757348900	3.776871310	-2.503298400
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C	-4.150490170	-0.365626420	-1.247864340
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C	2.391886850	-3.411616720	-1.247864340
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C	0.365626420	4.150490170	1.247864340
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C	1.757348900	-3.776871310	2.503298400
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C	-3.410344450	-2.392192050	2.503298400
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C	3.418515960	-2.392725790	3.752957930
C	2.392725790	-3.418515960	3.752957930
C	-0.362903330	-4.156884560	3.752957930
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C	-3.781419300	-1.764158770	3.752957930
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C	-3.418515960	2.392725790	3.752957930
C	-2.392725790	3.418515960	3.752957930
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C	3.413266650	2.392126450	4.999049770
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C	1.759912400	-3.778275600	4.999049770
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C	-3.451824230	-2.413341530	12.505022250
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C	-1.782696710	3.815927190	12.505022250
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C	-2.490652600	3.468746590	13.721254670
C	0.422595130	4.249348970	13.721254670
C	1.758696370	3.891341720	13.721254670
C	3.891341720	1.758696370	13.721254670
C	4.249348970	0.422595130	13.721254670
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C	2.490652600	-3.468746590	13.721254670
C	-0.422595130	-4.249348970	13.721254670
C	-1.758696370	-3.891341720	13.721254670
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H	-2.158915750	3.895034900	-14.676676820
H	-0.077841570	4.452657050	-14.676676820
H	2.293741300	3.817193330	-14.676676820
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H	4.452657050	-0.077841570	-14.676676820
H	3.895034900	-2.158915750	-14.676676820
H	2.158915750	-3.895034900	-14.676676820
H	0.077841570	-4.452657050	-14.676676820
H	-2.293741300	-3.817193330	-14.676676820
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H	-4.452657050	0.077841570	-14.676676820
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H	-3.895034900	2.158915750	14.676676820
H	-2.158915750	3.895034900	14.676676820
H	-0.077841570	4.452657050	14.676676820
H	2.293741300	3.817193330	14.676676820
H	3.817193330	2.293741300	14.676676820
H	4.452657050	-0.077841570	14.676676820
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Nanotube (6,6) u12v0s
B3LYP/STO-3G Energy: -10856.533290

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C	1.438122130	3.954815020	-13.134677280
C	2.705915840	3.222867360	-13.134899760
C	4.144031340	0.731957210	-13.134677280
C	4.144042920	-0.731958170	-13.134899760
C	2.705909210	-3.222857810	-13.134677280
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C	2.661394680	3.180742390	-10.635045970
C	4.085301680	0.714450560	-10.635011220
C	4.085301050	-0.714464210	-10.635045970
C	2.661383170	-3.180749750	-10.635011220
C	1.423906370	-3.895206600	-10.635045970
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C	3.909586430	1.425232690	-9.378244320
C	3.909580420	-1.425246430	-9.378316350
C	3.189080930	-2.673184830	-9.378244320
C	0.720490600	-4.098419170	-9.378316350
C	-0.720505500	-4.098417510	-9.378244320
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C	-4.104083230	0.721439470	-3.130379030
C	-2.676828180	3.193518650	-3.130346720
C	-1.427256710	3.914960070	-3.130379030
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C	-3.191661610	2.672129340	-1.875440350
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C	0.721441880	4.104082370	3.130346720
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C	-3.914960530	-1.427254190	3.130346720
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H	-4.330805970	-1.082215290	-15.306796310
H	-4.291695630	-1.228177050	15.306796310
H	-4.291702850	1.228209360	15.306865750
H	-3.209480340	3.102628920	15.306796310
H	-1.082190910	4.330828370	15.306865750
H	1.082215290	4.330805970	15.306796310
H	3.209511930	3.102619010	15.306865750
H	4.291695630	1.228177050	15.306796310
H	4.291702850	-1.228209360	15.306865750
H	3.209480340	-3.102628920	15.306796310

H	1.082190910	-4.330828370	15.306865750
H	-1.082215290	-4.330805970	15.306796310
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Nanotube (6,6) ul2v6s
B3LYP/STO-3G Energy: -11308.319976

C	-3.89817903	1.76221817	14.95892278
C	-4.25703116	0.42296381	14.95892278
C	-3.47521522	-2.49481298	14.95892278
C	-2.49481298	-3.47521522	14.95892278
C	0.42296381	-4.25703116	14.95892278
C	1.76221817	-3.89817903	14.95892278
C	3.89817903	-1.76221817	14.95892278
C	4.25703116	-0.42296381	14.95892278
C	3.47521522	2.49481298	14.95892278
C	2.49481298	3.47521522	14.95892278
C	-0.42296381	4.25703116	14.95892278
C	-1.76221817	3.89817903	14.95892278
C	-4.20151360	-0.36288705	13.74699580
C	-3.82006104	-1.78648740	13.74699580
C	-1.78648740	-3.82006104	13.74699580
C	-0.36288705	-4.20151360	13.74699580
C	2.41502620	-3.45717399	13.74699580
C	3.45717399	-2.41502620	13.74699580
C	4.20151360	0.36288705	13.74699580
C	3.82006104	1.78648740	13.74699580
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C	0.36288705	4.20151360	13.74699580
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C	-3.45717399	2.41502620	13.74699580
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C	-2.38419280	-3.41026945	12.50710914
C	0.35963680	-4.14547638	12.50710914
C	1.76128358	-3.76990626	12.50710914
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C	3.39675793	-2.38437513	11.24433822
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C	-2.39019199	-3.41654879	9.99319474
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C	3.78128000	1.76315861	8.75048769
C	1.76315861	3.78128000	8.75048769
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C	1.76463455	3.78295775	6.24488659
C	0.36326052	4.15845479	6.24488659
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C	-3.41969723	2.39382023	6.24488659
C	-4.15845479	-0.36326052	6.24488659
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C	-4.15666417	0.36371156	5.00109222
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C	-3.41127372	2.39274517	3.74826483
C	-4.15062228	-0.36654124	3.74826483
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C	0.42296381	-4.25703116	-14.95892278
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H	0.07523232	4.45865788	15.91592767
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H	-3.82369483	2.29448203	-15.91592767
H	-4.45865788	-0.07523232	-15.91592767
H	-3.89892715	-2.16417584	-15.91592767
H	-2.16417584	-3.89892715	-15.91592767
H	-0.07523232	-4.45865788	-15.91592767
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H	3.82369483	-2.29448203	-15.91592767
H	4.45865788	0.07523232	-15.91592767
H	3.89892715	2.16417584	-15.91592767
H	2.16417584	3.89892715	-15.91592767
H	0.07523232	4.45865788	-15.91592767
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Nanotube (6,6) ul3v0s
B3LYP/STO-3G Energy: -11760.097655

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C	-3.30182057	2.70507614	-15.59636437
C	-0.69175467	4.21199950	-15.59637561
C	0.69175437	4.21199857	-15.59636437
C	3.30182123	2.70507687	-15.59637561
C	3.99357494	1.50692243	-15.59636437
C	3.99357590	-1.50692263	-15.59637561
C	3.30182057	-2.70507614	-15.59636437
C	0.69175467	-4.21199950	-15.59637561
C	-0.69175437	-4.21199857	-15.59636437
C	-3.30182123	-2.70507687	-15.59637561

C	-3.99357494	-1.50692243	-15.59636437
C	-2.70936626	3.22375284	-14.38050329
C	-1.43716952	3.95825528	-14.38049300
C	1.43716872	3.95825643	-14.38050329
C	2.70936487	3.22375295	-14.38049300
C	4.14653499	0.73450359	-14.38050329
C	4.14653439	-0.73450233	-14.38049300
C	2.70936626	-3.22375284	-14.38050329
C	1.43716952	-3.95825528	-14.38049300
C	-1.43716872	-3.95825643	-14.38050329
C	-2.70936487	-3.22375295	-14.38049300
C	-4.14653499	-0.73450359	-14.38050329
C	-4.14653439	0.73450233	-14.38049300
C	-0.72605271	4.09747505	-13.14025852
C	0.72605004	4.09747566	-13.14025739
C	3.18549112	2.67751762	-13.14025852
C	3.91154303	1.41996005	-13.14025739
C	3.91154384	-1.41995743	-13.14025852
C	3.18549299	-2.67751561	-13.14025739
C	0.72605271	-4.09747505	-13.14025852
C	-0.72605004	-4.09747566	-13.14025739
C	-3.18549112	-2.67751762	-13.14025852
C	-3.91154303	-1.41996005	-13.14025739
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C	-3.18549299	2.67751561	-13.14025739
C	1.42403383	3.89638766	-11.87911455
C	2.66235240	3.18144422	-11.87912627
C	4.08638761	0.71494436	-11.87911455
C	4.08638771	-0.71494270	-11.87912627
C	2.66235378	-3.18144330	-11.87911455
C	1.42403532	-3.89638692	-11.87912627
C	-1.42403383	-3.89638766	-11.87911455
C	-2.66235240	-3.18144422	-11.87912627
C	-4.08638761	-0.71494436	-11.87911455
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C	-2.66235378	3.18144330	-11.87911455
C	-1.42403532	3.89638692	-11.87912627
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C	3.91420779	-1.42449234	-10.62481760
C	3.19074984	-2.67755703	-10.62483472
C	0.72345735	-4.10204955	-10.62481760
C	-0.72345749	-4.10204893	-10.62483472
C	-3.19075045	-2.67755722	-10.62481760
C	-3.91420733	-1.42449190	-10.62483472
C	-3.91420779	1.42449234	-10.62481760
C	-3.19074984	2.67755703	-10.62483472
C	-0.72345735	4.10204955	-10.62481760
C	0.72345749	4.10204893	-10.62483472
C	4.10820962	0.72506124	-9.38122210
C	4.10820974	-0.72506265	-9.38123216
C	2.68202626	-3.19528327	-9.38122210
C	1.42618219	-3.92034533	-9.38123216
C	-1.42618335	-3.92034451	-9.38122210
C	-2.68202755	-3.19528267	-9.38123216
C	-4.10820962	-0.72506124	-9.38122210
C	-4.10820974	0.72506265	-9.38123216
C	-2.68202626	3.19528327	-9.38122210
C	-1.42618219	3.92034533	-9.38123216
C	1.42618335	3.92034451	-9.38122210
C	2.68202755	3.19528267	-9.38123216
C	3.91248098	-1.42866036	-8.12881310
C	3.19349581	-2.67397870	-8.12880926
C	0.71898433	-4.10263810	-8.12881310
C	-0.71898558	-4.10263785	-8.12880926
C	-3.19349665	-2.67397774	-8.12881310
C	-3.91248139	-1.42865915	-8.12880926
C	-3.91248098	1.42866036	-8.12881310
C	-3.19349581	2.67397870	-8.12880926
C	-0.71898433	4.10263810	-8.12881310

C	0.71898558	4.10263785	-8.12880926
C	3.19349665	2.67397774	-8.12881310
C	3.91248139	1.42865915	-8.12880926
C	2.67933821	-3.19526956	-6.87398353
C	1.42751329	-3.91800974	-6.87396736
C	-1.42751550	-3.91800973	-6.87398353
C	-2.67933932	-3.19526764	-6.87396736
C	-4.10685371	-0.72274018	-6.87398353
C	-4.10685261	0.72274210	-6.87396736
C	-2.67933821	3.19526956	-6.87398353
C	-1.42751329	3.91800974	-6.87396736
C	1.42751550	3.91800973	-6.87398353
C	2.67933932	3.19526764	-6.87396736
C	4.10685371	0.72274018	-6.87398353
C	4.10685261	-0.72274210	-6.87396736
C	0.72542633	-4.11037181	-5.62838032
C	-0.72542485	-4.11037278	-5.62836060
C	-3.19697324	-2.68342354	-5.62838032
C	-3.92239967	-1.42695004	-5.62836060
C	-3.92239957	1.42694828	-5.62838032
C	-3.19697482	2.68342274	-5.62836060
C	-0.72542633	4.11037181	-5.62838032
C	0.72542485	4.11037278	-5.62836060
C	3.19697324	2.68342354	-5.62838032
C	3.92239967	1.42695004	-5.62836060
C	3.92239957	-1.42694828	-5.62838032
C	3.19697482	-2.68342274	-5.62836060
C	-1.42824854	-3.91403353	-4.37844946
C	-2.67552779	-3.19391677	-4.37843175
C	-4.10377674	-0.72011724	-4.37844946
C	-4.10377695	0.72011664	-4.37843175
C	-2.67552819	3.19391628	-4.37844946
C	-1.42824917	3.91403342	-4.37843175
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C	4.10377674	0.72011724	-4.37844946
C	4.10377695	-0.72011664	-4.37843175
C	2.67552819	-3.19391628	-4.37844946
C	1.42824917	-3.91403342	-4.37843175
C	-3.19420517	-2.67749757	-3.12334301
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C	-3.91588349	1.42751404	-3.12334301
C	-3.19420399	2.67749815	-3.12332424
C	-0.72167833	4.10501160	-3.12334301
C	0.72167942	4.10501088	-3.12332424
C	3.19420517	2.67749757	-3.12334301
C	3.91588341	1.42751273	-3.12332424
C	3.91588349	-1.42751404	-3.12334301
C	3.19420399	-2.67749815	-3.12332424
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C	-0.72167942	-4.10501088	-3.12332424
C	-4.10967235	-0.72535824	-1.87617277
C	-4.10967343	0.72535724	-1.87615242
C	-2.68301484	3.19640154	-1.87617277
C	-1.42665892	3.92176022	-1.87615242
C	1.42665751	3.92175978	-1.87617277
C	2.68301452	3.19640297	-1.87615242
C	4.10967235	0.72535824	-1.87617277
C	4.10967343	-0.72535724	-1.87615242
C	2.68301484	-3.19640154	-1.87617277
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C	-0.72094799	4.10470604	-0.62766643
C	0.72094703	4.10470540	-0.62764799
C	3.19430571	2.67671230	-0.62766643
C	3.91525266	1.42799425	-0.62764799
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C	3.19430563	-2.67671114	-0.62764799
C	0.72094799	-4.10470604	-0.62766643
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C	-2.67671114	3.19430563	0.62764799
C	-1.42799374	3.91525370	0.62766643
C	1.42799425	3.91525266	0.62764799
C	2.67671230	3.19430571	0.62766643
C	4.10470540	0.72094703	0.62764799
C	4.10470604	-0.72094799	0.62766643
C	2.67671114	-3.19430563	0.62764799
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C	-1.42799425	-3.91525266	0.62764799
C	-2.67671230	-3.19430571	0.62766643
C	-4.10470540	-0.72094703	0.62764799
C	-4.10470604	0.72094799	0.62766643
C	-0.72535724	4.10967343	1.87615242
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C	3.92175978	1.42665751	1.87617277
C	3.92176022	-1.42665892	1.87615242
C	3.19640154	-2.68301484	1.87617277
C	0.72535724	-4.10967343	1.87615242
C	-0.72535824	-4.10967235	1.87617277
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C	-3.92175978	-1.42665751	1.87617277
C	-3.92176022	1.42665892	1.87615242
C	-3.19640154	2.68301484	1.87617277
C	1.42751273	3.91588341	3.12332424
C	2.67749757	3.19420517	3.12334301
C	4.10501088	0.72167942	3.12332424
C	4.10501160	-0.72167833	3.12334301
C	2.67749815	-3.19420399	3.12332424
C	1.42751404	-3.91588349	3.12334301
C	-1.42751273	-3.91588341	3.12332424
C	-2.67749757	-3.19420517	3.12334301
C	-4.10501088	-0.72167942	3.12332424
C	-4.10501160	0.72167833	3.12334301
C	-2.67749815	3.19420399	3.12332424
C	-1.42751404	3.91588349	3.12334301
C	3.19391677	2.67552779	4.37843175
C	3.91403353	1.42824854	4.37844946
C	3.91403342	-1.42824917	4.37843175
C	3.19391628	-2.67552819	4.37844946
C	0.72011664	-4.10377695	4.37843175
C	-0.72011724	-4.10377674	4.37844946
C	-3.19391677	-2.67552779	4.37843175
C	-3.91403353	-1.42824854	4.37844946
C	-3.91403342	1.42824917	4.37843175
C	-3.19391628	2.67552819	4.37844946
C	-0.72011664	4.10377695	4.37843175
C	0.72011724	4.10377674	4.37844946
C	4.11037278	0.72542485	5.62836060
C	4.11037181	-0.72542633	5.62838032
C	2.68342274	-3.19697482	5.62836060
C	1.42694828	-3.92239957	5.62838032
C	-1.42695004	-3.92239967	5.62836060
C	-2.68342354	-3.19697324	5.62838032
C	-4.11037278	-0.72542485	5.62836060
C	-4.11037181	0.72542633	5.62838032
C	-2.68342274	3.19697482	5.62836060
C	-1.42694828	3.92239957	5.62838032
C	1.42695004	3.92239967	5.62836060
C	2.68342354	3.19697324	5.62838032
C	3.91800974	-1.42751329	6.87396736
C	3.19526956	-2.67933821	6.87398353
C	0.72274210	-4.10685261	6.87396736
C	-0.72274018	-4.10685371	6.87398353
C	-3.19526764	-2.67933932	6.87396736

C	-3.91800973	-1.42751550	6.87398353
C	-3.91800974	1.42751329	6.87396736
C	-3.19526956	2.67933821	6.87398353
C	-0.72274210	4.10685261	6.87396736
C	0.72274018	4.10685371	6.87398353
C	3.19526764	2.67933932	6.87396736
C	3.91800973	1.42751550	6.87398353
C	2.67397870	-3.19349581	8.12880926
C	1.42866036	-3.91248098	8.12881310
C	-1.42865915	-3.91248139	8.12880926
C	-2.67397774	-3.19349665	8.12881310
C	-4.10263785	-0.71898558	8.12880926
C	-4.10263810	0.71898433	8.12881310
C	-2.67397870	3.19349581	8.12880926
C	-1.42866036	3.91248098	8.12881310
C	1.42865915	3.91248139	8.12880926
C	2.67397774	3.19349665	8.12881310
C	4.10263785	0.71898558	8.12880926
C	4.10263810	-0.71898433	8.12881310
C	0.72506265	-4.10820974	9.38123216
C	-0.72506124	-4.10820962	9.38122210
C	-3.19528267	-2.68202755	9.38123216
C	-3.92034451	-1.42618335	9.38122210
C	-3.92034533	1.42618219	9.38123216
C	-3.19528327	2.68202626	9.38122210
C	-0.72506265	4.10820974	9.38123216
C	0.72506124	4.10820962	9.38122210
C	3.19528267	2.68202755	9.38123216
C	3.92034451	1.42618335	9.38122210
C	3.92034533	-1.42618219	9.38123216
C	3.19528327	-2.68202626	9.38122210
C	-1.42449190	-3.91420733	10.62483472
C	-2.67755722	-3.19075045	10.62481760
C	-4.10204893	-0.72345749	10.62483472
C	-4.10204955	0.72345735	10.62481760
C	-2.67755703	3.19074984	10.62483472
C	-1.42449234	3.91420779	10.62481760
C	1.42449190	3.91420733	10.62483472
C	2.67755722	3.19075045	10.62481760
C	4.10204893	0.72345749	10.62483472
C	4.10204955	-0.72345735	10.62481760
C	2.67755703	-3.19074984	10.62483472
C	1.42449234	-3.91420779	10.62481760
C	-3.18144422	-2.66235240	11.87912627
C	-3.89638766	-1.42403383	11.87911455
C	-3.89638692	1.42403532	11.87912627
C	-3.18144330	2.66235378	11.87911455
C	-0.71494270	4.08638771	11.87912627
C	0.71494436	4.08638761	11.87911455
C	3.18144422	2.66235240	11.87912627
C	3.89638766	1.42403383	11.87911455
C	3.89638692	-1.42403532	11.87912627
C	3.18144330	-2.66235378	11.87911455
C	0.71494270	-4.08638771	11.87912627
C	-0.71494436	-4.08638761	11.87911455
C	-4.09747566	-0.72605004	13.14025739
C	-4.09747505	0.72605271	13.14025852
C	-2.67751561	3.18549299	13.14025739
C	-1.41995743	3.91154384	13.14025852
C	1.41996005	3.91154303	13.14025739
C	2.67751762	3.18549112	13.14025852
C	4.09747566	0.72605004	13.14025739
C	4.09747505	-0.72605271	13.14025852
C	2.67751561	-3.18549299	13.14025739
C	1.41995743	-3.91154384	13.14025852
C	-1.41996005	-3.91154303	13.14025739
C	-2.67751762	-3.18549112	13.14025852
C	-3.95825528	1.43716952	14.38049300
C	-3.22375284	2.70936626	14.38050329
C	-0.73450233	4.14653439	14.38049300

C	0.73450359	4.14653499	14.38050329
C	3.22375295	2.70936487	14.38049300
C	3.95825643	1.43716872	14.38050329
C	3.95825528	-1.43716952	14.38049300
C	3.22375284	-2.70936626	14.38050329
C	0.73450233	-4.14653439	14.38049300
C	-0.73450359	-4.14653499	14.38050329
C	-3.22375295	-2.70936487	14.38049300
C	-3.95825643	-1.43716872	14.38050329
C	-2.70507614	3.30182057	15.59636437
C	-1.50692263	3.99357590	15.59637561
C	1.50692243	3.99357494	15.59636437
C	2.70507687	3.30182123	15.59637561
C	4.21199857	0.69175437	15.59636437
C	4.21199950	-0.69175467	15.59637561
C	2.70507614	-3.30182057	15.59636437
C	1.50692263	-3.99357590	15.59637561
C	-1.50692243	-3.99357494	15.59636437
C	-2.70507687	-3.30182123	15.59637561
C	-4.21199857	-0.69175437	15.59636437
C	-4.21199950	0.69175467	15.59637561
H	-4.31786761	1.07566827	-16.55211660
H	-3.09048834	3.20154893	-16.55212034
H	-1.22737776	4.27721717	-16.55211660
H	1.22737854	4.27721588	-16.55212034
H	3.09048985	3.20154890	-16.55211660
H	4.31786687	1.07566694	-16.55212034
H	4.31786761	-1.07566827	-16.55211660
H	3.09048834	-3.20154893	-16.55212034
H	1.22737776	-4.27721717	-16.55211660
H	-1.22737854	-4.27721588	-16.55212034
H	-3.09048985	-3.20154890	-16.55211660
H	-4.31786687	-1.07566694	-16.55212034
H	-3.20154893	3.09048834	16.55212034
H	-1.07566827	4.31786761	16.55211660
H	1.07566694	4.31786687	16.55212034
H	3.20154890	3.09048985	16.55211660
H	4.27721588	1.22737854	16.55212034
H	4.27721717	-1.22737776	16.55211660
H	3.20154893	-3.09048834	16.55212034
H	1.07566827	-4.31786761	16.55211660
H	-1.07566694	-4.31786687	16.55212034
H	-3.20154890	-3.09048985	16.55211660
H	-4.27721588	-1.22737854	16.55212034
H	-4.27721717	1.22737776	16.55211660

Nanotube (6,6) ul3v6s
B3LYP/STO-3G Energy: -12211.867269

C	-3.46523844	2.48861980	-16.22981278
C	-2.48861980	3.46523844	-16.22981278
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C	1.75667462	3.88782719	-16.22981278
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H	4.34315436	-1.08996190	17.78503506
H	4.34312877	1.08998345	17.78506205
H	3.11551187	3.21630106	17.78503506
H	1.22761103	4.30625157	17.78506205
H	-1.22764249	4.30626296	17.78503506
H	-3.21630106	-3.11551187	-17.78503506
H	-1.08998345	-4.34312877	-17.78506205
H	1.08996190	-4.34315436	-17.78503506
H	3.21626812	-3.11551774	-17.78506205
H	4.30626296	-1.22764249	-17.78503506
H	4.30625157	1.22761103	-17.78506205
H	3.21630106	3.11551187	-17.78503506
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Nanotube (6,6) u14v6s
B3LYP/STO-3G Energy: -13115.429629

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C	3.88977908	1.75858122	-17.47044737
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C	-0.36348802	4.19539377	-16.25487185
C	2.41248674	3.45157357	-16.25487185
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C	4.19539377	-0.36348802	-16.25487185
C	3.81506159	-1.78290703	-16.25487185
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C	0.36348802	-4.19539377	-16.25487185
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C	-3.45157357	-2.41248674	-16.25487185
C	-4.19539377	0.36348802	-16.25487185
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C	1.76158247	3.76955855	-15.01460971
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C	4.14532470	0.35920410	-15.01460971
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C	4.13245058	-0.36701145	-13.75319570
C	3.76231291	-1.74838405	-13.75319570
C	1.74838405	-3.76231291	-13.75319570
C	0.36701145	-4.13245058	-13.75319570
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C	-0.36272173	-4.15020199	-12.49928333
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C	-2.38922722	3.41281949	-12.49928333
C	0.36272173	4.15020199	-12.49928333
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C	0.36472366	-4.15533133	-8.74869649
C	-2.39352562	-3.41626066	-8.74869649
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B3LYP/STO-3G Energy: -14018.982338

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Nanotube (6,6) ul6v0s
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Nanotube (6,6) ul6v6s
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Nanotube (6,6) u17v0s
B3LYP/STO-3G Energy: -15374.313428

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Nanotube (6,6) u17v6s
B3LYP/STO-3G Energy: -15826.093167

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Nanotube (6,6) u18v6s
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C	1.76051181	-3.89180221	-22.45979968
C	3.89180221	-1.76051181	-22.45979968
C	4.25065549	-0.42125315	-22.45979968
C	3.47054906	2.49014368	-22.45979968
C	2.49014368	3.47054906	-22.45979968
C	-0.42125315	4.25065549	-22.45979968
C	-1.76051181	3.89180221	-22.45979968
H	-3.81002485	2.29025767	23.41758032
H	-4.44470715	-0.07840889	23.41758032
H	-3.88843375	-2.15444948	23.41758032
H	-2.15444948	-3.88843375	23.41758032
H	-0.07840889	-4.44470715	23.41758032
H	2.29025767	-3.81002485	23.41758032
H	3.81002485	-2.29025767	23.41758032
H	4.44470715	0.07840889	23.41758032
H	3.88843375	2.15444948	23.41758032
H	2.15444948	3.88843375	23.41758032
H	0.07840889	4.44470715	23.41758032
H	-2.29025767	3.81002485	23.41758032
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H	-0.07840889	-4.44470715	-23.41758032
H	2.29025767	-3.81002485	-23.41758032
H	3.81002485	-2.29025767	-23.41758032
H	4.44470715	0.07840889	-23.41758032
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H	2.15444948	3.88843375	-23.41758032
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Nanotube (6,6) u19v0s
B3LYP/STO-3G Energy: -17181.424719

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C	-3.99513220	1.50713044	23.09335005
C	-3.99512484	-1.50712829	23.09331804
C	-3.30277935	-2.70632076	23.09335005
C	-0.69235103	-4.21344375	23.09331804
C	0.69235285	-4.21345120	23.09335005
C	3.30277381	-2.70631546	23.09331804
C	3.99513220	-1.50713044	23.09335005
C	3.99512484	1.50712829	23.09331804
C	3.30277935	2.70632076	23.09335005
C	0.69235103	4.21344375	23.09331804
C	-0.69235285	4.21345120	23.09335005
C	-4.14922149	0.73561941	21.87877808
C	-4.14922134	-0.73563299	21.87876913
C	-2.71167585	-3.22552151	21.87877808

C	-1.43753381	-3.96114758	21.87876913
C	1.43754565	-3.96114093	21.87877808
C	2.71168752	-3.22551459	21.87876913
C	4.14922149	-0.73561941	21.87877808
C	4.14922134	0.73563299	21.87876913
C	2.71167585	3.22552151	21.87877808
C	1.43753381	3.96114758	21.87876913
C	-1.43754565	3.96114093	21.87877808
C	-2.71168752	3.22551459	21.87876913
C	-3.91261663	-1.42070873	20.63880173
C	-3.18667195	-2.67807585	20.63872867
C	-0.72593847	-4.09877976	20.63880173
C	0.72594575	-4.09877679	20.63872867
C	3.18667817	-2.67807103	20.63880173
C	3.91261770	-1.42070094	20.63872867
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C	-0.72594575	4.09877679	20.63872867
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C	-3.91261770	1.42070094	20.63872867
C	-2.66377886	-3.18270660	19.37712787
C	-1.42441353	-3.89825450	19.37702880
C	1.42441534	-3.89825346	19.37712787
C	2.66378067	-3.18270555	19.37702880
C	4.08819420	-0.71554686	19.37712787
C	4.08819419	0.71554895	19.37702880
C	2.66377886	3.18270660	19.37712787
C	1.42441353	3.89825450	19.37702880
C	-1.42441534	3.89825346	19.37712787
C	-2.66378067	3.18270555	19.37702880
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C	-0.72459369	-4.10503243	18.12430521
C	0.72458747	-4.10503509	18.12424230
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C	3.91735841	-1.42500639	18.12424230
C	3.91735921	1.42499967	18.12430521
C	3.19277094	2.68002870	18.12424230
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C	-3.91735921	-1.42499967	18.12430521
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C	4.10868879	-0.72473774	16.88129334
C	4.10869019	0.72472763	16.88131448
C	2.68198569	3.19586000	16.88129334
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C	4.10742982	0.72376696	14.37470695
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C	-1.42691901	3.91901967	14.37460576
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C	-3.91860644	-1.42750928	10.62470680
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C	-3.19363251	2.67589205	8.12832259
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C	-1.42741370	-3.91713352	6.87413388
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C	2.67699807	-3.19449415	4.37748739
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C	1.42801405	3.91559540	4.37748739
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C	0.72197149	-4.10586286	3.12333813
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Nanotube (6,6) ul9v6s
B3LYP/STO-3G Energy: -17633.201055

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C	-3.195291000	-2.682095000	17.510064000
C	-0.725116000	4.108251000	17.510064000
C	2.674159000	3.193450000	16.258430000
C	-4.102688000	0.719164000	16.258430000
C	1.428530000	-3.912614000	16.258430000
C	-2.674159000	-3.193450000	16.258430000
C	4.102688000	-0.719164000	16.258430000
C	-1.428530000	3.912614000	16.258430000
C	2.674159000	-3.193450000	-16.258430000
C	-4.102688000	-0.719164000	-16.258430000
C	1.428530000	3.912614000	-16.258430000
C	-2.674159000	3.193450000	-16.258430000
C	4.102688000	0.719164000	-16.258430000
C	-1.428530000	-3.912614000	-16.258430000
C	-2.674159000	-3.193450000	-16.258430000
C	4.102688000	-0.719164000	-16.258430000
C	-1.428530000	3.912614000	-16.258430000
C	2.674159000	3.193450000	-16.258430000
C	-4.102688000	0.719164000	-16.258430000
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C	-3.916454000	-1.427520000	15.003364000
C	3.194496000	-2.677989000	15.003364000
C	-0.721958000	-4.105509000	15.003364000
C	3.916454000	1.427520000	15.003364000
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C	2.682627000	3.196067000	13.756777000
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C	3.914078000	1.427851000	12.507483000
C	3.193594000	-2.675765000	12.507483000
C	0.720484000	4.103616000	12.507483000
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C	0.722415000	-4.105903000	-5.004477000
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C	-2.674987000	-3.193172000	3.750795000
C	-4.102861000	0.720021000	3.750795000
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C	2.674987000	3.193172000	3.750795000
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C	-0.723878000	-4.107451000	2.499373000
C	-3.919096000	-1.426829000	2.499373000
C	3.195218000	-2.680622000	2.499373000
C	0.723878000	4.107451000	2.499373000
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C	-4.106823000	0.723217000	1.252647000
C	1.427087000	-3.918222000	1.252647000
C	-2.679736000	-3.195005000	1.252647000
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Nanotube (6,6) u20v0_
B3LYP/STO-3G Energy: -18084.975277

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H	3.40496778	-25.28911017	2.85829044
C	2.93052698	-24.33111910	3.10708258
H	-0.77289149	-25.28910387	4.37806654
C	-1.22556593	-24.33118098	4.09158544
H	-4.17809947	-25.28906681	1.51969531
C	-4.15623745	-24.33119435	0.98450441
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C	1.36397054	4.04517629	27.47552724
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H	3.56824179	2.65961355	-28.43143113
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H	4.08741380	-1.76038126	-28.43143113
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Nanotube (6,6) u23v6s
B3LYP/STO-3G Energy: -21247.419188

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C	-1.760739320	-3.779727750	8.748071150
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C	4.153902030	-0.363522730	19.996162390
C	3.779146050	-1.762131100	19.996162390
C	1.762131100	-3.779146050	19.996162390
C	0.363522730	-4.153902030	19.996162390
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C	0.424948510	4.263775840	28.705734470
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Nanotube (6,6) u24v0s
B3LYP/STO-3G Energy: -21699.195841

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C	-3.97567926	-1.38992130	28.13446254
C	-2.15792464	-3.61680476	28.13446895
C	-0.78413248	-4.13799989	28.13446254
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C	3.19154679	-2.74807859	28.13446254
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C	0.78413248	4.13799989	28.13446254
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C	-4.08958341	0.77493959	26.89433629
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C	-2.71590908	-3.15421333	26.89433629
C	-0.05972213	-4.16192619	26.89434399
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C	-4.14938957	0.05068135	25.63344983
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C	-2.11858613	-3.56813610	25.63344983
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C	-0.05669605	-4.16518447	24.37973072
C	1.37183327	-3.93320353	24.37970998
C	3.57880753	-2.13169246	24.37973072
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C	3.63044967	2.03817795	-25.00955391
C	2.71560152	3.15602781	-25.00956092
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C	-1.37539950	3.92979381	-25.00956092
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C	-0.36302917	-4.19175120	-30.00741789
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H	-0.08734733	-4.41141525	32.18262780
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H	3.77672401	-2.28135263	-32.18262780
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Nanotube (6,6) u26v0s
B3LYP/STO-3G Energy: -23506.301085

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6	1.424186	-3.897196	29.381091
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6	3.181803	-2.662894	-29.383065
6	3.897036	-1.424075	-29.383065
6	3.897036	1.424075	-29.383065
6	3.181803	2.662894	-29.383065
6	-1.420111	3.911425	-30.644366
6	-2.677338	3.185565	-30.644366
6	-4.097449	0.725861	-30.644366
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6	-2.677338	-3.185565	-30.644366
6	-1.420111	-3.911425	-30.644366
6	1.420111	-3.911425	-30.644366
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6	4.097449	0.725861	-30.644366
6	2.677338	3.185565	-30.644366
6	1.420111	3.911425	-30.644366
6	-3.223875	2.709772	-31.884683
6	-3.958669	1.437072	-31.884683
6	-3.958669	-1.437072	-31.884683
6	-3.223875	-2.709772	-31.884683
6	-0.734794	-4.146844	-31.884683
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6	3.223875	-2.709772	-31.884683
6	3.958669	-1.437072	-31.884683
6	3.958669	1.437072	-31.884683
6	3.223875	2.709772	-31.884683
6	0.734794	4.146844	-31.884683
6	-0.734794	4.146844	-31.884683
6	-4.211982	0.691997	-33.099994
6	-4.211982	-0.691997	-33.099994
6	-2.705278	-3.301685	-33.099994
6	-1.506704	-3.993682	-33.099994
6	1.506704	-3.993682	-33.099994
6	2.705278	-3.301685	-33.099994
6	4.211982	-0.691997	-33.099994
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1	3.089558	3.200504	34.056471
1	1.226939	4.275888	34.056471
1	-1.226939	4.275888	34.056471
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Nanotube (6,6) u27v6s
B3LYP/STO-3G Energy: -24861.632294

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C	1.76174298	-3.89518327	33.70938320
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C	-0.42187746	4.25419916	33.70938320
C	-1.76174298	3.89518327	33.70938320
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C	-3.82067646	-1.78704668	32.49716589
C	-1.78704668	-3.82067646	32.49716589
C	-0.36271041	-4.20232621	32.49716589
C	2.41527954	-3.45796605	32.49716589
C	3.45796605	-2.41527954	32.49716589
C	4.20232621	0.36271041	32.49716589
C	3.82067646	1.78704668	32.49716589
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C	0.36271041	4.20232621	32.49716589
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C	-3.45796605	2.41527954	32.49716589
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C	0.35958296	-4.14484495	31.25689823
C	1.76101450	-3.76933250	31.25689823
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C	4.14484495	-0.35958296	31.25689823
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C	-0.36637909	-4.13449578	29.99364859
C	2.38454149	-3.39738883	29.99364859
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C	4.13449578	0.36637909	29.99364859
C	3.76376792	1.74995429	29.99364859
C	1.74995429	3.76376792	29.99364859
C	0.36637909	4.13449578	29.99364859
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C	0.36151137	-4.15447852	28.74308610
C	1.76416123	-3.77863962	28.74308610
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C	0.35958296	-4.14484495	-31.25689823
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C	4.14484495	-0.35958296	-31.25689823
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C	-0.36271041	-4.20232621	-32.49716589
C	3.89518327	-1.76174298	-33.70938320
C	4.25419916	-0.42187746	-33.70938320
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C	-0.42187746	4.25419916	-33.70938320
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Nanotube (6,6) u28v0s
B3LYP/STO-3G Energy: -25313.417910

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C	2.681683	-3.195719	-28.128831
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Nanotube (6,6) u28v6s
B3LYP/STO-3G Energy: -25765.191056

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6	2.710545	-3.224543	-35.634034
6	4.147808	0.735129	-35.634034
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6	-3.994181	-1.506823	-36.849206
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6	3.994181	1.506823	-36.849206
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1	-3.089215	-3.200186	-37.805706
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1	-3.089215	3.200186	-37.805706
1	-4.316049	-1.075246	-37.805706
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6	4.103583	0.724141	31.879037
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C	0.36246741	-4.20048225	36.24345976
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C	-3.39803288	-2.38501940	33.74036813
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C	3.77879681	1.76416065	32.48978695
C	1.76416065	3.77879681	32.48978695
C	0.36159047	4.15461435	32.48978695
C	-2.39045371	3.41720634	32.48978695
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H	-4.44794452	0.07781416	-38.41365156
H	-3.81312587	-2.29136130	-38.41365156
H	-2.29136130	-3.81312587	-38.41365156
H	0.07781416	-4.44794452	-38.41365156
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Nanotube (6,6) u31v0s
B3LYP/STO-3G Energy: -28024.077238

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6	1.437283	3.961993	36.875742
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6	-4.149828	0.736273	36.875742
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6	-2.712545	-3.225720	36.875742
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6	3.186154	-2.677414	35.635582
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6	3.186154	2.677414	35.635582
6	0.725631	4.097998	35.635582
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6	4.109114	-0.724670	24.376660
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6	3.914904	-1.428020	23.125379
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6	3.194153	2.676396	23.125379
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6	2.713828	-3.226447	-38.118380
6	4.151099	-0.737021	-38.118380
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6	1.437271	3.963468	-38.118380
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6	3.303202	-2.707696	-39.331065
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6	3.303202	2.707696	-39.331065
6	0.693332	4.214505	-39.331065
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1	-3.198401	-3.087031	40.288770

1	-1.074247	-4.313411	40.288770
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6	-8.751157	-1.427246	-3.917603
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6	23.757801	-4.108649	-0.724658
6	23.757801	-4.108649	0.724658
6	23.757803	-2.681918	3.195884
6	23.757804	-1.426758	3.920522
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6	23.757803	2.681918	3.195884
6	23.757801	4.108649	0.724658
6	23.757801	4.108649	-0.724658
6	23.757803	2.681918	-3.195884
6	23.757804	1.426758	-3.920522
6	25.006635	-3.193963	-2.676801
6	25.006634	-3.915147	-1.427638
6	25.006634	-3.915147	1.427638
6	25.006635	-3.193963	2.676801
6	25.006636	-0.721197	4.104408
6	25.006636	0.721197	4.104408
6	25.006635	3.193963	2.676801
6	25.006634	3.915147	1.427638
6	25.006634	3.915147	-1.427638
6	25.006635	3.193963	-2.676801
6	25.006636	0.721197	-4.104408
6	25.006636	-0.721197	-4.104408
6	26.260965	-4.104432	-0.721106

6	26.260965	-4.104432	0.721106
6	26.260966	-2.676730	3.194003
6	26.260967	-1.427720	3.915087
6	26.260967	1.427720	3.915087
6	26.260966	2.676730	3.194003
6	26.260965	4.104432	0.721106
6	26.260965	4.104432	-0.721106
6	26.260966	2.676730	-3.194003
6	26.260967	1.427720	-3.915087
6	26.260967	-1.427720	-3.915087
6	26.260966	-2.676730	-3.194003
6	27.509839	-3.920865	1.426685
6	27.509841	-3.195994	2.682230
6	27.509843	-0.724882	4.108874
6	27.509843	0.724882	4.108874
6	27.509841	3.195994	2.682230
6	27.509839	3.920865	1.426685
6	27.509839	3.920865	-1.426685
6	27.509841	3.195994	-2.682230
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6	27.509843	-0.724882	-4.108874
6	27.509841	-3.195994	-2.682230
6	27.509839	-3.920865	-1.426685
6	28.757408	-2.677628	3.194196
6	28.757409	-1.427443	3.915956
6	28.757409	1.427443	3.915956
6	28.757408	2.677628	3.194196
6	28.757405	4.105056	0.721783
6	28.757405	4.105056	-0.721783
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6	28.757408	-2.677628	-3.194196
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6	30.011997	0.720295	4.103451
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6	30.011993	3.913889	1.427945
6	30.011993	3.913889	-1.427945
6	30.011993	3.193602	-2.675544
6	30.011997	0.720295	-4.103451
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6	30.011993	-3.193602	-2.675544
6	30.011993	-3.913889	-1.427945
6	30.011993	-3.913889	1.427945
6	30.011993	-3.193602	2.675544
6	31.262160	1.426725	3.921245
6	31.262159	2.682580	3.196216
6	31.262159	4.109290	0.725057
6	31.262159	4.109290	-0.725057
6	31.262159	2.682580	-3.196216
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6	31.262159	-4.109290	0.725057
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6	31.262160	-1.426725	3.921245
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6	32.508195	3.195114	-2.679222
6	32.508194	0.722727	-4.106588
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6	33.762605	1.428593	-3.912673
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6	35.014992	3.195455	-2.681946
6	35.014992	0.724919	-4.108239
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6	36.258682	2.677906	-3.191196
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6	37.512702	-3.181789	-2.662678
6	37.512713	-3.896870	-1.424132
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6	37.512702	-3.181789	2.662678
6	37.512696	-0.715070	4.086778
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6	38.773804	-1.420166	-3.911824
6	38.773802	-2.677699	-3.185833
6	38.773835	-4.097865	-0.726023
6	38.773835	-4.097865	0.726023
6	38.773802	-2.677699	3.185833
6	38.773804	-1.420166	3.911824
6	38.773804	1.420166	3.911824
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6	38.773835	4.097865	-0.726023
6	38.773802	2.677699	-3.185833
6	38.773804	1.420166	-3.911824
6	40.014117	-3.224063	-2.709719
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6	40.014117	-3.224063	2.709719
6	40.014113	-0.734636	4.146903
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6	40.014117	3.224063	2.709719
6	40.014144	3.958654	1.437259
6	40.014144	3.958654	-1.437259

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6	41.229931	-4.211889	-0.691852
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6	41.229870	-2.705221	3.301890
6	41.229871	-1.506882	3.993714
6	41.229871	1.506882	3.993714
6	41.229870	2.705221	3.301890
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6	41.229870	2.705221	-3.301890
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1	-42.186179	4.275879	1.226824
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1	-42.186107	3.200604	-3.089970
1	-42.186106	1.075665	-4.316771
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Nanotube (6,6) u34v0s
B3LYP/STO-3G Energy: -30734.740115

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C	2.712438	-3.225646	-40.623359
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C	3.911736	-1.420565	-39.383308

C	3.186134	-2.677425	-39.383305
C	0.725635	-4.097999	-39.383336
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C	-3.186134	-2.677425	-39.383305
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C	-2.664102	-3.182744	-38.121101
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C	-2.664102	3.182744	-38.121101
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C	3.917940	1.424582	-36.869394
C	3.917940	-1.424582	-36.869394
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C	3.194413	-2.676630	-26.873566
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Nanotube (6,6) u34v6s
B3LYP/STO-3G Energy: -31186.517206

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C	-0.363115	-4.155921	36.889399
C	-1.763497	-3.780709	36.889395
C	-3.780709	-1.763497	36.889395
C	-4.155921	-0.363115	36.889399
C	-3.417617	2.392472	36.889403
C	-2.392472	3.417617	36.889403
C	2.389408	3.412820	38.133002
C	3.412820	2.389408	38.133002
C	4.150252	-0.362868	38.133009
C	3.775672	-1.760882	38.133012
C	1.760882	-3.775673	38.133012
C	0.362868	-4.150252	38.133009
C	-2.389408	-3.412820	38.133002
C	-3.412820	-2.389408	38.133002
C	-4.150252	0.362868	38.133009
C	-3.775673	1.760882	38.133012
C	-1.760882	3.775672	38.133012
C	-0.362868	4.150252	38.133009
C	3.762577	1.748496	39.386882
C	4.132729	0.367038	39.386892
C	3.395543	-2.384251	39.386897
C	2.384251	-3.395543	39.386897
C	-0.367039	-4.132730	39.386892
C	-1.748497	-3.762578	39.386882
C	-3.762578	-1.748497	39.386882
C	-4.132730	-0.367039	39.386892
C	-3.395543	2.384251	39.386897
C	-2.384251	3.395543	39.386897
C	0.367038	4.132729	39.386892
C	1.748496	3.762577	39.386882
C	4.146041	-0.359320	40.648094
C	3.770246	-1.761828	40.648091
C	1.761827	-3.770246	40.648091
C	0.359320	-4.146041	40.648093
C	-2.384244	-3.410945	40.648069
C	-3.410945	-2.384244	40.648069
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C	-3.770246	1.761827	40.648091
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C	-0.359320	4.146041	40.648094
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C	3.410944	2.384244	40.648069
C	3.452008	-2.412968	41.888406
C	2.412967	-3.452009	41.888406
C	-0.363695	-4.195965	41.888405
C	-1.783068	-3.815699	41.888382
C	-3.815699	-1.783068	41.888382
C	-4.195965	-0.363695	41.888405
C	-3.452009	2.412967	41.888406
C	-2.412968	3.452008	41.888406
C	0.363694	4.195964	41.888405
C	1.783067	3.815699	41.888382
C	3.815699	1.783067	41.888382
C	4.195964	0.363694	41.888405
C	1.758524	-3.889462	43.104010
C	0.421774	-4.247605	43.104012
C	-2.489214	-3.467774	43.103976
C	-3.467774	-2.489214	43.103976
C	-4.247605	0.421774	43.104012
C	-3.889462	1.758524	43.104010
C	-1.758524	3.889461	43.104011
C	-0.421775	4.247604	43.104012
C	2.489214	3.467773	43.103977
C	3.467773	2.489214	43.103977
C	4.247604	-0.421775	43.104012
C	3.889461	-1.758524	43.104011
H	-3.812585	-2.291663	-44.060316

H	-4.447583	0.078375	-44.060318
H	-3.891099	2.156097	-44.060269
H	-2.156098	3.891098	-44.060269
H	-0.078376	4.447582	-44.060318
H	2.291662	3.812584	-44.060316
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H	4.447582	-0.078376	-44.060318
H	3.891098	-2.156098	-44.060269
H	2.156097	-3.891099	-44.060269
H	0.078375	-4.447583	-44.060318
H	-2.291663	-3.812585	-44.060316
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H	-0.078376	-4.447583	44.060318
H	-2.156098	-3.891099	44.060269
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H	-4.447583	-0.078376	44.060318
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H	2.156097	3.891098	44.060269
H	3.891098	2.156097	44.060269
H	4.447582	0.078375	44.060318
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Nanotube (6,6) u35v6s
B3LYP/STO-3G Energy: -32090.071140

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C	0.421252	-4.249134	43.712493
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C	4.249134	-0.421252	43.712493
C	3.469368	2.489539	43.712456
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C	-0.421252	4.249134	43.712493
C	-1.759734	3.890526	43.712492
C	-4.198751	-0.362830	42.498776
C	-3.817681	-1.785216	42.498752
C	-1.785216	-3.817681	42.498752
C	-0.362830	-4.198751	42.498776
C	2.413605	-3.454851	42.498778
C	3.454851	-2.413605	42.498778
C	4.198751	0.362830	42.498776
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C	-3.410603	-2.384490	41.258667
C	-2.384490	-3.410603	41.258667
C	0.359701	-4.145866	41.258693
C	1.761406	-3.770284	41.258691
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C	4.145866	-0.359701	41.258693
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C	-4.145866	0.359701	41.258693
C	-1.749566	-3.763659	39.996314
C	-0.366655	-4.134200	39.996324
C	2.384650	-3.397006	39.996330
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C	3.763659	1.749566	39.996314
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C	0.366655	4.134200	39.996324
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C	-3.763659	-1.749567	39.996314
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C	1.763163	-3.777723	38.744728
C	3.777722	-1.763163	38.744728
C	4.153169	-0.361917	38.744724
C	3.415823	2.390045	38.744717
C	2.390045	3.415823	38.744717
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C	-1.763163	3.777722	38.744728
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C	3.780767	1.763031	37.501604
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C	0.363547	4.155739	37.501607
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C	-3.780767	-1.763031	37.501603
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C	-0.363547	-4.155739	37.501607
C	3.777867	-1.757341	36.247455
C	4.150374	-0.367033	36.247452
C	3.410843	2.393075	36.247449
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C	-0.367033	4.150374	36.247452
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C	-3.781803	1.763505	33.750587
C	-4.156862	0.363666	33.750586
C	-3.418149	-2.393403	33.750583
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C	4.156862	-0.363666	33.750586
C	1.758109	3.777899	32.498145
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C	-4.151305	0.366102	28.748560
C	-3.412115	-2.392736	28.748561
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C	0.366102	-4.151305	28.748560
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C	4.151305	-0.366102	28.748560
C	3.412116	2.392737	28.748560
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C	-0.366102	4.151305	28.748560
C	-1.758611	3.778208	28.748560
C	-4.155484	-0.364105	27.496065
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C	2.393286	-3.418134	22.499783
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C	0.363563	4.156779	22.499783
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C	-0.363563	-4.156778	22.499783
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C	-4.156722	0.363605	-26.249893
C	-3.418061	-2.393286	-26.249893
C	-2.393286	-3.418061	-26.249893
C	0.363605	-4.156722	-26.249893
C	1.763484	-3.781650	-26.249892
C	3.781650	-1.763484	-26.249892
C	4.156722	-0.363605	-26.249893
C	1.762422	3.780826	-27.496065
C	0.364104	4.155484	-27.496065
C	-2.393110	3.416743	-27.496065
C	-3.416742	2.393110	-27.496065
C	-4.155484	-0.364105	-27.496065
C	-3.780826	-1.762422	-27.496065
C	-1.762422	-3.780826	-27.496065
C	-0.364105	-4.155484	-27.496065
C	2.393110	-3.416743	-27.496065
C	3.416743	-2.393110	-27.496065
C	4.155484	0.364104	-27.496065
C	3.780826	1.762422	-27.496065
C	-0.366102	4.151305	-28.748560
C	-1.758611	3.778208	-28.748560
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C	-4.151305	0.366102	-28.748560
C	-3.412115	-2.392736	-28.748561
C	-2.392736	-3.412115	-28.748561
C	0.366102	-4.151305	-28.748560
C	1.758611	-3.778208	-28.748560
C	3.778208	-1.758611	-28.748560
C	4.151305	-0.366102	-28.748560
C	3.412115	2.392736	-28.748561
C	2.392736	3.412115	-28.748561
C	-2.393262	3.417984	-30.000116
C	-3.417984	2.393262	-30.000116
C	-4.156633	-0.363615	-30.000116
C	-3.781576	-1.763419	-30.000116
C	-1.763419	-3.781576	-30.000116
C	-0.363615	-4.156633	-30.000116
C	2.393262	-3.417984	-30.000116
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C	4.156632	0.363615	-30.000116
C	3.781575	1.763419	-30.000116
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C	0.363615	4.156632	-30.000117
C	-3.781112	1.762904	-31.245767
C	-4.155965	0.363840	-31.245767
C	-3.417286	-2.393107	-31.245767
C	-2.393107	-3.417286	-31.245767
C	0.363840	-4.155965	-31.245767
C	1.762904	-3.781112	-31.245767
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C	-4.150796	-0.366372	-32.498146
C	-3.777899	-1.758109	-32.498145
C	-1.758109	-3.777899	-32.498145
C	-0.366372	-4.150796	-32.498146
C	2.392732	-3.411547	-32.498147
C	3.411547	-2.392732	-32.498147
C	4.150796	0.366372	-32.498146
C	3.777899	1.758109	-32.498145
C	1.758109	3.777899	-32.498145

C	0.366372	4.150796	-32.498146
C	-2.392732	3.411547	-32.498147
C	-3.411547	2.392732	-32.498147
C	-3.418149	-2.393403	-33.750583
C	-2.393403	-3.418149	-33.750583
C	0.363666	-4.156862	-33.750586
C	1.763506	-3.781802	-33.750587
C	3.781802	-1.763506	-33.750587
C	4.156862	-0.363666	-33.750586
C	3.418149	2.393403	-33.750584
C	2.393403	3.418149	-33.750584
C	-0.363666	4.156862	-33.750586
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C	-4.156862	0.363666	-33.750586
C	-1.763890	-3.782163	-34.995395
C	-0.363500	-4.157377	-34.995397
C	2.393537	-3.418688	-34.995400
C	3.418688	-2.393537	-34.995400
C	4.157377	0.363500	-34.995397
C	3.782163	1.763890	-34.995395
C	1.763890	3.782163	-34.995395
C	0.363500	4.157377	-34.995397
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C	-3.418688	2.393537	-34.995400
C	-4.157377	-0.363500	-34.995397
C	-3.782163	-1.763890	-34.995395
C	0.367033	-4.150374	-36.247452
C	1.757341	-3.777867	-36.247455
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C	4.150374	-0.367033	-36.247452
C	3.410843	2.393075	-36.247449
C	2.393075	3.410843	-36.247449
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C	2.392753	-3.417240	-37.501612
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C	4.155739	0.363547	-37.501607
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C	-0.363547	-4.155739	-37.501607
C	3.777722	-1.763163	-38.744728
C	4.153169	-0.361917	-38.744725
C	3.415823	2.390045	-38.744717
C	2.390045	3.415823	-38.744717
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C	4.134200	0.366655	-39.996324
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C	3.397006	-2.384651	-39.996331
C	3.410603	2.384489	-41.258668
C	2.384489	3.410603	-41.258668
C	-0.359701	4.145866	-41.258693
C	-1.761406	3.770284	-41.258691
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C	-4.145867	0.359701	-41.258693
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C	4.145866	-0.359701	-41.258693
C	1.785216	3.817680	-42.498752
C	0.362830	4.198751	-42.498776
C	-2.413605	3.454851	-42.498778
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C	-4.198751	-0.362830	-42.498776
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C	4.198751	0.362830	-42.498776
C	3.817681	1.785216	-42.498752
C	-0.421252	4.249134	-43.712494
C	-1.759735	3.890525	-43.712492
C	-3.890526	1.759734	-43.712492
C	-4.249135	0.421252	-43.712493
C	-3.469368	-2.489539	-43.712455
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C	0.421252	-4.249134	-43.712493
C	1.759734	-3.890526	-43.712492
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C	4.249134	-0.421252	-43.712494
C	3.469368	2.489539	-43.712456
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H	-3.810152	2.290760	44.669725
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H	-3.889122	-2.154457	44.669675
H	-2.154457	-3.889122	44.669675
H	-0.078817	-4.445032	44.669726
H	2.290760	-3.810152	44.669725
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H	4.445032	0.078817	44.669726
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H	2.154456	3.889121	44.669675
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H	-4.445032	-0.078817	-44.669726
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H	-2.154457	-3.889122	-44.669675
H	-0.078817	-4.445032	-44.669726
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Nanotube (6,6) u36v0s
B3LYP/STO-3G Energy: -32541.850349

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C	0.421521	-4.248313	-44.346477
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C	-3.453483	2.413309	-43.131836
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C	1.784181	3.816745	-43.131810
C	3.816745	1.784181	-43.131810
C	4.197422	0.363260	-43.131834
C	3.453483	-2.413308	-43.131836
C	2.413309	-3.453483	-43.131836
C	-0.363260	-4.197422	-43.131834
C	-1.784181	-3.816744	-43.131810
C	-3.816744	-1.784180	-43.131810
C	-4.197422	-0.363260	-43.131834
C	-1.761697	3.770406	-41.891733
C	-0.359507	4.146119	-41.891735
C	2.384452	3.410921	-41.891709
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C	4.146119	-0.359507	-41.891735
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C	1.761697	-3.770405	-41.891733
C	0.359508	-4.146118	-41.891735
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C	-4.146118	0.359508	-41.891735
C	-3.770405	1.761697	-41.891733
C	0.366851	4.133571	-40.629952
C	1.749085	3.763213	-40.629942
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C	4.133571	0.366851	-40.629952
C	3.396363	-2.384502	-40.629959
C	2.384503	-3.396363	-40.629960
C	-0.366850	-4.133571	-40.629952
C	-1.749084	-3.763212	-40.629942
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C	-4.133571	-0.366850	-40.629952
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C	3.776864	-1.762135	-39.377206
C	1.762135	-3.776864	-39.377206
C	0.362377	-4.151913	-39.377202
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C	-4.151913	0.362377	-39.377202
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C	-0.362376	4.151913	-39.377202
C	3.780851	1.763342	-38.133951
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C	3.417551	-2.392669	-38.133961
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C	-0.363320	-4.155965	-38.133955
C	-1.763342	-3.780850	-38.133951
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C	0.363409	-4.157069	-34.382164
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C	-0.366426	-4.150327	-33.130674
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C	1.757827	3.777521	-33.130673
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C	-4.154290	0.364470	-31.877091
C	-3.779978	1.761521	-31.877091
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C	-0.364470	4.154290	-31.877091
C	2.392815	3.415520	-31.877091
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C	4.154290	-0.364470	-31.877091
C	3.779978	-1.761521	-31.877091
C	1.761521	-3.779978	-31.877091
C	0.364470	-4.154290	-31.877091
C	-3.781657	-1.763750	-30.630826
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C	-2.393169	3.418313	-30.630826
C	0.363369	4.156869	-30.630826
C	1.763750	3.781657	-30.630826
C	3.781657	1.763750	-30.630826

C	4.156869	0.363369	-30.630826
C	3.418313	-2.393169	-30.630826
C	2.393169	-3.418313	-30.630826
C	-0.363369	-4.156869	-30.630826
C	-1.763750	-3.781657	-30.630826
C	-4.151098	0.366070	-29.380459
C	-3.778013	1.758536	-29.380460
C	-1.758536	3.778013	-29.380459
C	-0.366070	4.151098	-29.380459
C	2.392605	3.411953	-29.380459
C	3.411953	2.392605	-29.380459
C	4.151098	-0.366070	-29.380459
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C	-4.153642	-0.364811	-28.126797
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C	4.156279	0.363638	11.875989
C	3.417664	-2.393099	11.875989
C	2.393099	-3.417664	11.875989
C	-2.392657	-3.412930	13.125738
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C	-4.151962	0.365622	13.125738
C	-3.778536	1.759350	13.125738
C	-1.759350	3.778536	13.125738
C	-0.365622	4.151962	13.125738
C	2.392657	3.412929	13.125738

C	3.412929	2.392657	13.125738
C	4.151962	-0.365622	13.125738
C	3.778536	-1.759350	13.125738
C	1.759350	-3.778536	13.125738
C	0.365622	-4.151962	13.125738
C	-3.779429	-1.760576	14.378882
C	-4.153348	-0.365008	14.378882
C	-3.414438	2.392818	14.378882
C	-2.392818	3.414438	14.378882
C	0.365008	4.153348	14.378882
C	1.760576	3.779429	14.378882
C	3.779429	1.760576	14.378882
C	4.153348	0.365007	14.378882
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C	2.392818	-3.414438	14.378882
C	-0.365008	-4.153348	14.378882
C	-1.760576	-3.779429	14.378882
C	-4.156520	0.363531	15.626862
C	-3.781438	1.763442	15.626862
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C	-0.363531	4.156520	15.626862
C	2.393127	3.417926	15.626862
C	3.417926	2.393127	15.626862
C	4.156520	-0.363531	15.626862
C	3.781438	-1.763443	15.626862
C	1.763442	-3.781438	15.626862
C	0.363531	-4.156520	15.626862
C	-2.393127	-3.417927	15.626862
C	-3.417926	-2.393127	15.626862
C	-3.413265	2.392684	16.875978
C	-2.392684	3.413265	16.875978
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C	1.759628	3.778728	16.875977
C	3.778728	1.759628	16.875977
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C	-1.760102	3.779102	18.129365
C	-0.365254	4.152828	18.129365
C	2.392772	3.413864	18.129364
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C	-4.152828	0.365254	18.129365
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C	0.363453	4.156702	19.377770
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C	3.418122	-2.393149	19.377771
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C	-0.363453	-4.156702	19.377770
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C	-2.393149	3.418122	19.377771
C	2.392718	3.413683	20.626234
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C	-1.759972	3.778963	20.626234
C	-0.365297	4.152643	20.626234
C	3.778766	1.759615	21.879790
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C	3.413271	-2.392722	21.879790
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C	-0.365509	-4.152292	21.879790
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C	0.365509	4.152292	21.879790
C	1.759615	3.778766	21.879790
C	4.156823	-0.363401	23.128719
C	3.781635	-1.763704	23.128719
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C	0.363401	-4.156823	23.128719
C	-2.393168	-3.418255	23.128718
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C	-0.363401	4.156823	23.128719
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C	-0.365081	-4.153098	24.376508
C	-1.760390	-3.779249	24.376508
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C	3.779249	1.760390	24.376508
C	4.153098	0.365081	24.376508
C	1.759100	-3.778409	25.630158
C	0.365772	-4.151729	25.630158
C	-2.392675	-3.412654	25.630157
C	-3.412654	-2.392675	25.630157
C	-4.151729	0.365772	25.630158
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C	-0.363381	-4.156889	26.879723
C	-1.763762	-3.781683	26.879723
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C	-4.156889	-0.363381	26.879723
C	-3.418318	2.393176	26.879723
C	-2.393176	3.418319	26.879723
C	0.363381	4.156889	26.879723
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C	2.393176	-3.418318	26.879723
C	-2.392801	-3.414794	28.126797
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C	-4.153642	0.364811	28.126797

C	-3.779584	1.760888	28.126797
C	-1.760888	3.779584	28.126797
C	-0.364811	4.153642	28.126797
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C	-3.778013	-1.758536	29.380460
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C	0.366070	4.151098	29.380459
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C	-4.156869	0.363369	30.630826
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C	-0.363369	4.156869	30.630826
C	2.393169	3.418313	30.630826
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C	-3.415519	2.392815	31.877091
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C	1.761521	3.779978	31.877091
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C	-3.779978	-1.761521	31.877091
C	-4.154290	-0.364470	31.877091
C	-1.757827	3.777521	33.130673
C	-0.366426	4.150327	33.130673
C	2.392546	3.411115	33.130674
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C	4.150327	-0.366426	33.130673
C	3.777521	-1.757827	33.130673
C	1.757827	-3.777521	33.130673
C	0.366426	-4.150327	33.130674
C	-2.392545	-3.411114	33.130674
C	-3.411114	-2.392545	33.130674
C	-4.150327	0.366426	33.130674
C	-3.777521	1.757827	33.130673
C	0.363409	4.157069	34.382164
C	1.763832	3.781854	34.382166
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C	4.157069	0.363409	34.382164
C	3.418459	-2.393285	34.382162
C	2.393285	-3.418458	34.382162
C	-0.363409	-4.157069	34.382164
C	-1.763832	-3.781853	34.382166
C	-3.781853	-1.763832	34.382166
C	-4.157069	-0.363409	34.382164
C	-3.418458	2.393285	34.382162
C	-2.393285	3.418459	34.382162
C	2.393264	3.417146	35.627337

C	3.417146	2.393264	35.627337
C	4.155905	-0.364034	35.627334
C	3.781156	-1.762691	35.627331
C	1.762691	-3.781156	35.627331
C	0.364034	-4.155905	35.627334
C	-2.393264	-3.417146	35.627337
C	-3.417146	-2.393264	35.627337
C	-4.155905	0.364034	35.627334
C	-3.781156	1.762692	35.627331
C	-1.762691	3.781156	35.627331
C	-0.364034	4.155905	35.627333
C	3.777435	1.756906	36.880556
C	4.149782	0.367193	36.880553
C	3.410251	-2.392919	36.880549
C	2.392920	-3.410251	36.880549
C	-0.367193	-4.149782	36.880553
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C	-3.777435	-1.756906	36.880556
C	-4.149782	-0.367193	36.880553
C	-3.410251	2.392920	36.880549
C	-2.392919	3.410251	36.880549
C	0.367193	4.149782	36.880553
C	1.756906	3.777435	36.880556
C	4.155966	-0.363320	38.133955
C	3.780851	-1.763342	38.133951
C	1.763342	-3.780850	38.133951
C	0.363321	-4.155965	38.133955
C	-2.392669	-3.417550	38.133961
C	-3.417550	-2.392669	38.133961
C	-4.155966	0.363321	38.133955
C	-3.780850	1.763342	38.133951
C	-1.763342	3.780851	38.133951
C	-0.363320	4.155966	38.133955
C	2.392670	3.417551	38.133960
C	3.417551	2.392670	38.133960
C	3.414506	-2.389817	39.377194
C	2.389817	-3.414506	39.377194
C	-0.362376	-4.151913	39.377202
C	-1.762135	-3.776864	39.377206
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C	-4.151913	-0.362376	39.377202
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C	4.151913	0.362377	39.377202
C	1.749085	-3.763212	40.629942
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C	-2.384502	-3.396363	40.629960
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C	-3.763212	1.749085	40.629942
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C	-0.366850	4.133571	40.629952
C	2.384503	3.396363	40.629959
C	3.396363	2.384503	40.629959
C	4.133571	-0.366850	40.629952
C	3.763213	-1.749084	40.629942
C	-0.359507	-4.146118	41.891735
C	-1.761697	-3.770405	41.891733
C	-3.770405	-1.761696	41.891733
C	-4.146119	-0.359507	41.891735
C	-3.410920	2.384452	41.891709
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C	3.770406	1.761697	41.891733
C	4.146119	0.359508	41.891735
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C	2.384452	-3.410920	41.891709
C	-2.413308	-3.453483	43.131836
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C	-4.197422	0.363260	43.131834
C	-3.816745	1.784181	43.131810
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C	-0.363260	4.197422	43.131834
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C	1.784181	-3.816744	43.131810
C	0.363260	-4.197422	43.131834
C	-3.889948	-1.759085	44.346476
C	-4.248313	-0.421521	44.346477
C	-3.468520	2.489364	44.346439
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C	0.421521	4.248313	44.346477
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C	3.889949	1.759086	44.346476
C	4.248313	0.421521	44.346477
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H	-4.446507	-0.078607	-45.303297
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H	0.078607	4.446508	-45.303297
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H	4.446507	0.078607	-45.303297
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H	-0.078607	-4.446507	-45.303297
H	-2.155376	-3.890289	-45.303246
H	-3.890289	-2.155376	-45.303246
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H	-3.890289	2.155376	45.303246
H	-2.155376	3.890289	45.303246
H	-0.078607	4.446507	45.303297
H	2.291308	3.811534	45.303296
H	3.811534	2.291309	45.303296
H	4.446507	-0.078607	45.303297
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H	2.155376	-3.890289	45.303246
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Nanotube (6,6) u36v6s
B3LYP/STO-3G Energy: -32993.626767

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C	0.691911	4.212187	-44.977618
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C	3.994103	1.507013	-44.977543
C	3.994103	-1.507000	-44.977544
C	3.302201	-2.705429	-44.977548
C	0.691911	-4.212174	-44.977620
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C	-3.302199	-2.705429	-44.977548
C	-3.994101	-1.507000	-44.977545
C	-3.994101	1.507013	-44.977544
C	-3.302199	2.705442	-44.977546
C	1.437299	3.958957	-43.762008
C	2.710012	3.224249	-43.761975
C	4.147269	0.734781	-43.761965

C	4.147269	-0.734768	-43.761965
C	2.710012	-3.224237	-43.761977
C	1.437299	-3.958945	-43.762010
C	-1.437298	-3.958945	-43.762010
C	-2.710011	-3.224237	-43.761978
C	-4.147267	-0.734768	-43.761966
C	-4.147267	0.734781	-43.761965
C	-2.710011	3.224249	-43.761976
C	-1.437298	3.958957	-43.762008
C	3.185902	2.677720	-42.521732
C	3.911909	1.420197	-42.521730
C	3.911909	-1.420185	-42.521731
C	3.185902	-2.677709	-42.521734
C	0.726025	-4.097872	-42.521776
C	-0.726023	-4.097872	-42.521776
C	-3.185900	-2.677709	-42.521734
C	-3.911908	-1.420185	-42.521731
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C	-3.185900	2.677720	-42.521732
C	-0.726023	4.097883	-42.521774
C	0.726024	4.097883	-42.521774
C	4.087004	0.715175	-41.260536
C	4.087004	-0.715164	-41.260536
C	2.662869	-3.181883	-41.260550
C	1.424143	-3.897050	-41.260566
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C	-2.662868	-3.181883	-41.260550
C	-4.087003	-0.715164	-41.260537
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C	2.662869	3.181894	41.260547
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C	-0.726023	4.097884	42.521773
C	0.726024	4.097884	42.521773
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C	3.911909	-1.420185	42.521731
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C	4.147269	0.734782	43.761965
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C	2.710012	-3.224236	43.761978
C	1.437299	-3.958944	43.762011
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Nanotube (6,6) u37v0s
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C	1.748206	-3.762222	-41.894028
C	0.367111	-4.132276	-41.894037
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H	4.448624	-0.078301	-46.567428
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Nanotube (6,6) u37v6s
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1	-1.304072	-4.252070	47.177083
1	0.843189	-4.366871	47.177108
1	3.030364	-3.255395	47.177083
1	4.203416	-1.453213	47.177108
1	4.334436	0.996675	47.177083
1	-0.843189	4.366871	-47.177108
1	-3.030364	3.255395	-47.177083
1	-4.203416	1.453213	-47.177108
1	-4.334436	-0.996675	-47.177083
1	-3.360227	-2.913659	-47.177108
1	-1.304072	-4.252070	-47.177083
1	0.843189	-4.366871	-47.177108
1	3.030364	-3.255395	-47.177083
1	4.203416	-1.453213	-47.177108

1	4.334436	0.996675	-47.177083
1	3.360227	2.913659	-47.177108
1	1.304072	4.252070	-47.177083

Nanotube (6,6) u38v0s
B3LYP/STO-3G Energy: -34348.958317

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C	4.247720	0.421745	-46.847028
C	3.467893	-2.489248	-46.846992
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C	-0.421740	-4.247715	-46.847029
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C	-4.247715	-0.421740	-46.847029
C	-1.783666	3.816165	-45.631371
C	-0.363406	4.196667	-45.631394
C	2.413069	3.452760	-45.631395
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C	4.196667	-0.363406	-45.631394
C	3.816165	-1.783666	-45.631371
C	1.783671	-3.816160	-45.631371
C	0.363410	-4.196662	-45.631395
C	-2.413064	-3.452756	-45.631396
C	-3.452756	-2.413064	-45.631396
C	-4.196662	0.363410	-45.631395
C	-3.816160	1.783671	-45.631371
C	0.359361	4.145968	-44.391516
C	1.761757	3.770201	-44.391514
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C	4.145968	0.359361	-44.391516
C	3.410862	-2.384238	-44.391492
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C	-0.359356	-4.145963	-44.391517
C	-1.761752	-3.770197	-44.391515
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C	2.384252	3.395663	-43.129904
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C	4.132835	-0.366977	-43.129898
C	3.762640	-1.748598	-43.129889
C	1.748602	-3.762636	-43.129889
C	0.366981	-4.132831	-43.129899
C	-2.384248	-3.395659	-43.129905
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C	-0.366977	4.132835	-43.129898
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C	3.413735	-2.389752	-41.876613
C	2.389755	-3.413732	-41.876613
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C	-1.761498	-3.776425	-41.876624
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C	0.362711	4.151217	-41.876620
C	1.761502	3.776429	-41.876623
C	4.155906	-0.363213	-40.633374

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C	1.763404	-3.780742	-40.633372
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C	3.779815	-1.761334	-10.624927
C	1.761331	-3.779817	-10.624927
C	0.364545	-4.154062	-10.624927
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Nanotube (6,6) u39v0s
B3LYP/STO-3G Energy: -35252.513613

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6	-0.363414	-4.156883	30.628309
6	-1.763730	-3.781694	30.628309
6	-3.781694	-1.763730	30.628309
6	-4.156883	-0.363414	30.628309
6	-3.418297	2.393202	30.628309
6	-2.393202	3.418297	30.628309
6	2.392857	3.415152	31.875159
6	3.415152	2.392857	31.875159
6	4.153981	-0.364681	31.875159
6	3.779813	-1.761171	31.875159
6	1.761171	-3.779813	31.875159
6	0.364681	-4.153981	31.875159
6	-2.392857	-3.415152	31.875159
6	-3.415152	-2.392857	31.875159
6	-4.153981	0.364681	31.875159
6	-3.779813	1.761171	31.875159
6	-1.761171	3.779813	31.875159
6	-0.364681	4.153981	31.875159
6	3.778033	1.758525	33.128602
6	4.151111	0.366089	33.128602
6	3.411955	-2.392629	33.128602
6	2.392629	-3.411955	33.128602
6	-0.366089	-4.151111	33.128602
6	-1.758525	-3.778033	33.128602
6	-3.778033	-1.758525	33.128602
6	-4.151111	-0.366089	33.128602
6	-3.411955	2.392629	33.128602
6	-2.392629	3.411955	33.128602
6	0.366089	4.151111	33.128602
6	1.758525	3.778033	33.128602
6	4.156838	-0.363412	34.379159
6	3.781652	-1.763699	34.379159
6	1.763699	-3.781652	34.379159
6	0.363412	-4.156838	34.379159
6	-2.393189	-3.418265	34.379159
6	-3.418265	-2.393189	34.379159
6	-4.156838	0.363412	34.379159
6	-3.781652	1.763699	34.379159
6	-1.763699	3.781652	34.379159
6	-0.363412	4.156838	34.379159
6	2.393189	3.418265	34.379159
6	3.418264	2.393189	34.379159
6	3.415842	-2.392865	35.625262
6	2.392864	-3.415842	35.625262
6	-0.364351	-4.154593	35.625262
6	-1.761775	-3.780180	35.625262
6	-3.780180	-1.761775	35.625262
6	-4.154593	-0.364351	35.625262
6	-3.415842	2.392864	35.625262
6	-2.392865	3.415842	35.625262
6	0.364351	4.154593	35.625262
6	1.761775	3.780180	35.625262
6	3.780180	1.761775	35.625262
6	4.154593	0.364351	35.625262
6	1.757854	-3.777566	36.878610
6	0.366426	-4.150379	36.878611
6	-2.392570	-3.411159	36.878612
6	-3.411159	-2.392570	36.878612
6	-4.150379	0.366426	36.878611
6	-3.777566	1.757854	36.878610
6	-1.757854	3.777566	36.878610
6	-0.366426	4.150379	36.878611
6	2.392570	3.411159	36.878612

6	3.411159	2.392570	36.878612
6	4.150379	-0.366426	36.878611
6	3.777566	-1.757854	36.878610
6	-0.363450	-4.157021	38.130261
6	-1.763772	-3.781833	38.130262
6	-3.781833	-1.763772	38.130262
6	-4.157021	-0.363450	38.130261
6	-3.418397	2.393297	38.130259
6	-2.393297	3.418397	38.130259
6	0.363450	4.157021	38.130261
6	1.763772	3.781833	38.130262
6	3.781833	1.763772	38.130262
6	4.157021	0.363450	38.130261
6	3.418397	-2.393297	38.130259
6	2.393297	-3.418397	38.130259
6	-2.393313	-3.417429	39.375327
6	-3.417429	-2.393313	39.375327
6	-4.156174	0.363935	39.375324
6	-3.781340	1.762912	39.375322
6	-1.762912	3.781340	39.375322
6	-0.363935	4.156174	39.375324
6	2.393313	3.417428	39.375327
6	3.417428	2.393313	39.375327
6	4.156174	-0.363935	39.375324
6	3.781340	-1.762912	39.375322
6	1.762912	-3.781340	39.375322
6	0.363935	-4.156174	39.375324
6	-3.777499	-1.756971	40.628317
6	-4.149870	-0.367169	40.628315
6	-3.410339	2.392942	40.628311
6	-2.392943	3.410339	40.628311
6	0.367169	4.149870	40.628315
6	1.756970	3.777499	40.628317
6	3.777499	1.756970	40.628317
6	4.149870	0.367169	40.628315
6	3.410339	-2.392943	40.628311
6	2.392942	-3.410339	40.628311
6	-0.367169	-4.149870	40.628315
6	-1.756971	-3.777499	40.628317
6	-4.155929	0.363366	41.881841
6	-3.780842	1.763283	41.881838
6	-1.763283	3.780841	41.881838
6	-0.363367	4.155929	41.881841
6	2.392692	3.417496	41.881845
6	3.417496	2.392692	41.881845
6	4.155929	-0.363367	41.881841
6	3.780841	-1.763283	41.881838
6	1.763283	-3.780841	41.881838
6	0.363366	-4.155929	41.881841
6	-2.392692	-3.417496	41.881845
6	-3.417496	-2.392692	41.881845
6	-3.414743	2.389849	43.125025
6	-2.389850	3.414742	43.125025
6	0.362288	4.152135	43.125032
6	1.762325	3.777013	43.125035
6	3.777013	1.762325	43.125035
6	4.152135	0.362288	43.125032
6	3.414742	-2.389850	43.125025
6	2.389849	-3.414743	43.125025
6	-0.362288	-4.152135	43.125032
6	-1.762325	-3.777013	43.125035
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6	-4.152135	-0.362288	43.125032
6	-1.749163	3.763271	44.377566
6	-0.366809	4.133662	44.377576
6	2.384516	3.396464	44.377582
6	3.396464	2.384516	44.377582
6	4.133662	-0.366809	44.377576
6	3.763271	-1.749163	44.377566
6	1.749163	-3.763271	44.377566

6	0.366809	-4.133662	44.377576
6	-2.384516	-3.396464	44.377582
6	-3.396464	-2.384516	44.377582
6	-4.133662	0.366809	44.377576
6	-3.763271	1.749163	44.377566
6	0.359553	4.146111	45.639453
6	1.761658	3.770422	45.639450
6	3.770422	1.761658	45.639450
6	4.146111	0.359553	45.639453
6	3.410889	-2.384482	45.639428
6	2.384482	-3.410889	45.639428
6	-0.359553	-4.146111	45.639453
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6	-3.770422	-1.761658	45.639450
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6	-3.410889	2.384482	45.639428
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6	2.413435	3.453854	46.879571
6	3.453854	2.413435	46.879571
6	4.197800	-0.363179	46.879571
6	3.817030	-1.784434	46.879548
6	1.784434	-3.817030	46.879548
6	0.363178	-4.197800	46.879571
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6	-4.197800	0.363178	46.879571
6	-3.817030	1.784434	46.879548
6	-1.784434	3.817030	46.879548
6	-0.363179	4.197800	46.879571
6	3.890439	1.759339	48.093993
6	4.248860	0.421554	48.093995
6	3.468970	-2.489652	48.093960
6	2.489652	-3.468970	48.093960
6	-0.421554	-4.248860	48.093995
6	-1.759339	-3.890439	48.093993
6	-3.890439	-1.759339	48.093993
6	-4.248860	-0.421554	48.093995
6	-3.468970	2.489652	48.093960
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6	0.421554	4.248860	48.093995
6	1.759339	3.890439	48.093993
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1	-3.811720	2.291217	-49.050864
1	-2.291217	3.811720	-49.050864
1	0.078425	4.446617	-49.050866
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1	3.890279	2.155568	-49.050818
1	4.446617	0.078425	-49.050866
1	3.811720	-2.291217	-49.050864
1	2.291217	-3.811720	-49.050864
1	-0.078425	-4.446617	-49.050866
1	-2.155568	-3.890279	-49.050818
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1	3.811720	2.291217	49.050864
1	4.446616	-0.078425	49.050866
1	3.890279	-2.155568	49.050818
1	2.155568	-3.890279	49.050818
1	0.078425	-4.446617	49.050866
1	-2.291217	-3.811720	49.050864
1	-3.811720	-2.291217	49.050864
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1	-2.155568	3.890279	49.050818
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Nanotube (6,6) u39v6s
B3LYP/STO-3G Energy: -35704.282867

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C	4.214503	-0.693415	-48.702780
C	2.707884	-3.303359	-48.702723
C	1.506837	-3.996756	-48.702727
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C	-2.707880	-3.303359	-48.702724
C	-4.214498	-0.693415	-48.702781
C	-4.214498	0.693418	-48.702781
C	-2.707880	3.303362	-48.702723
C	-1.506833	3.996759	-48.702727
C	3.226573	2.714026	-47.490191
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C	3.226573	-2.714024	-47.490191
C	0.737116	-4.151239	-47.490193
C	-0.737112	-4.151239	-47.490193
C	-3.226568	-2.714024	-47.490192
C	-3.963636	-1.437278	-47.490217
C	-3.963636	1.437280	-47.490217
C	-3.226568	2.714026	-47.490191
C	-0.737112	4.151242	-47.490192
C	0.737116	4.151242	-47.490192
C	4.097877	0.725359	-46.250119
C	4.097877	-0.725357	-46.250119
C	2.677127	-3.186176	-46.250088
C	1.420750	-3.911508	-46.250092
C	-1.420746	-3.911508	-46.250093
C	-2.677123	-3.186176	-46.250089
C	-4.097873	-0.725357	-46.250120
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C	-2.677123	3.186179	-46.250088
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C	3.899566	-1.424239	-44.987252
C	3.183230	-2.664960	-44.987241
C	0.716329	-4.089181	-44.987238
C	-0.716325	-4.089181	-44.987238
C	-3.183227	-2.664960	-44.987241
C	-3.899562	-1.424239	-44.987253
C	-3.899562	1.424242	-44.987252
C	-3.183227	2.664963	-44.987241
C	-0.716325	4.089183	-44.987237
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C	3.899566	1.424242	-44.987252
C	2.682249	-3.193481	-43.736890
C	1.424535	-3.919591	-43.736889
C	-1.424531	-3.919591	-43.736889
C	-2.682246	-3.193481	-43.736891
C	-4.106776	-0.726131	-43.736895
C	-4.106776	0.726133	-43.736895
C	-2.682246	3.193483	-43.736890
C	-1.424531	3.919593	-43.736889
C	1.424535	3.919593	-43.736889
C	2.682249	3.193483	-43.736890
C	4.106780	0.726133	-43.736894
C	4.106780	-0.726131	-43.736894
C	0.724133	-4.108339	-42.493820
C	-0.724129	-4.108339	-42.493821
C	-3.195922	-2.681307	-42.493819
C	-3.920051	-1.427072	-42.493822
C	-3.920051	1.427074	-42.493822
C	-3.195922	2.681309	-42.493819
C	-0.724129	4.108341	-42.493820
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C	3.195925	2.681309	-42.493818

C	3.920054	1.427074	-42.493821
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C	3.195925	-2.681307	-42.493818
C	-1.428833	-3.915065	-41.238988
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C	-2.676165	3.194955	-41.238988
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C	2.676168	-3.194954	-41.238987
C	1.428835	-3.915065	-41.238988
C	-3.197652	-2.684230	-39.988344
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C	-3.197652	2.684232	-39.988343
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C	3.197655	2.684232	-39.988342
C	3.923443	1.427116	-39.988343
C	3.923443	-1.427115	-39.988343
C	3.197655	-2.684230	-39.988343
C	0.725794	-4.111302	-39.988343
C	-0.725791	-4.111302	-39.988343
C	-4.109333	-0.724235	-38.743613
C	-4.109333	0.724237	-38.743612
C	-2.681886	3.196664	-38.743611
C	-1.427454	3.920876	-38.743612
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C	2.681888	-3.196663	-38.743611
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C	-3.194721	-2.676828	-37.490278
C	-3.915564	-1.428273	-37.490277
C	-2.683154	3.196929	-36.239407
C	-1.427048	3.922112	-36.239408
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C	2.683156	3.196929	-36.239406
C	4.110192	0.725204	-36.239404
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C	2.683156	-3.196928	-36.239407
C	1.427050	-3.922111	-36.239408
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C	-2.683154	-3.196928	-36.239407
C	-4.110190	-0.725203	-36.239405
C	-4.110191	0.725204	-36.239405
C	-0.724154	4.109048	-34.993908
C	0.724156	4.109048	-34.993908
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C	3.920653	1.427400	-34.993904
C	3.920653	-1.427399	-34.993904
C	3.196505	-2.681682	-34.993905
C	0.724156	-4.109047	-34.993909

C	-0.724154	-4.109047	-34.993909
C	-3.196504	-2.681682	-34.993906
C	-3.920651	-1.427399	-34.993905
C	-3.920651	1.427400	-34.993905
C	-3.196504	2.681683	-34.993906
C	1.428183	3.916087	-33.741291
C	2.677362	3.194903	-33.741290
C	4.105535	0.721205	-33.741288
C	4.105535	-0.721204	-33.741288
C	2.677362	-3.194902	-33.741290
C	1.428183	-3.916087	-33.741291
C	-1.428182	-3.916087	-33.741291
C	-2.677361	-3.194902	-33.741290
C	-4.105534	-0.721204	-33.741289
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C	-2.677361	3.194903	-33.741290
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C	2.681683	-3.196513	-31.244479
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C	-1.427419	3.920636	-31.244479
C	1.427420	3.920636	-31.244479
C	2.681683	3.196514	-31.244478
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Nanotube (6,6) u40v0s
B3LYP/STO-3G Energy: -36156.064276

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Nanotube (6,6) u40v6_
B3LYP/STO-3G Energy: -36607.845686

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Nanotube (6,6) u41v0_
B3LYP/STO-3G Energy: -37059.619891

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Nanotube (6,6) u41v6_
B3LYP/STO-3G Energy: -37511.397228

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C	-0.36385887	-4.15573151	-13.75458218
C	-3.41703963	2.39297678	-13.75458218
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C	2.39297678	-3.41703963	-13.75458218
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C	0.36555441	-4.15184772	12.50575678
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C	-3.77838280	1.75934446	12.50575678
C	-0.36555441	4.15184772	12.50575678
C	-3.41282840	-2.39250326	12.50575678
C	3.77838280	-1.75934446	12.50575678
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Nanotube (7,5) u05v00
B3LYP/STO-3G Energy: -4531.654068

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6	-5.436361	1.339640	-3.601157
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6	-4.236281	-4.157491	1.151338
6	-3.980481	-3.654319	2.511481
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6	-4.281444	2.130895	-3.350537
6	-3.557163	-1.466827	4.327933
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6	-3.178904	3.588552	2.380691
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6	-1.905027	3.855714	1.734420
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6	-0.922702	-0.241110	4.275517
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6	2.984844	1.559331	3.666630
6	2.428699	-2.177263	-3.801304
6	2.643041	-3.263175	-2.863727
6	3.105433	3.683949	1.781194
6	3.129930	4.143683	0.403721
6	3.149621	-4.162929	-0.215128
6	3.410683	-3.886937	1.187708
6	3.178903	3.588740	-2.380412
6	3.214194	2.649833	-3.488081
6	3.862799	-2.044390	3.298636
6	4.027904	-0.685473	3.785257
6	3.418111	-0.001487	-4.546789
6	3.557162	-1.466478	-4.328053
6	4.281441	2.130629	3.350711

6	4.326878	3.281365	2.412590
6	3.980486	-3.654110	-2.511771
6	4.236287	-4.157388	-1.151665
6	4.383240	4.231616	-0.299313
6	4.405158	3.973973	-1.742556
6	4.760371	-3.657191	1.631426
6	4.992567	-2.735534	2.743655
6	4.483444	2.155201	-3.964730
6	4.551252	0.854989	-4.542782
6	5.334120	-0.070807	3.756794
6	5.436357	1.339357	3.601277
6	4.840798	-2.114998	-4.230826
6	5.043808	-3.182099	-3.365873
6	5.557619	3.735843	1.808077
6	5.585079	4.207608	0.505514
6	5.572909	-4.286496	-0.608919
6	5.824035	-4.060822	0.731961
6	5.643581	3.732498	-2.472239
6	5.682339	2.874921	-3.548980
6	6.318428	-2.218548	3.066186
6	6.485552	-0.949434	3.570346
1	-7.493842	-0.535153	-3.709669
1	-7.200734	-2.818279	-2.808556
1	-6.641560	2.620459	4.021281
1	-6.578610	4.163577	2.092194
1	-6.861946	-4.053402	-1.088850
1	-6.416436	-4.453393	1.290877
1	-6.552834	4.429162	-0.037597
1	-6.505427	3.593686	-2.343018
1	-6.061603	-3.568272	3.225899
1	-5.704270	-1.683787	4.753380
1	-6.434323	1.764196	-3.433637
1	-5.545731	0.443821	4.759173
1	5.545724	0.444202	-4.759146
1	6.434318	1.763928	3.433796
1	5.704265	-1.683411	-4.753531
1	6.061611	-3.568008	-3.226186
1	6.505423	3.593500	2.343303
1	6.552836	4.429151	0.037947
1	6.416442	-4.453269	-1.291227
1	6.861950	-4.053477	1.088535
1	6.578609	4.163734	-2.091866
1	6.641554	2.620783	-4.021085
1	7.200733	-2.818508	2.808363
1	7.493833	-0.535442	3.709663

Nanotube (7,5) u05v01
B3LYP/STO-3G Energy: -4606.949986

6	-6.267844	0.076868	-4.141242
6	-6.134861	-1.280793	-3.968162
6	-6.075656	1.941108	3.754883
6	-5.956628	3.046211	2.942855
6	-5.824377	-3.669196	-2.154647
6	-5.683220	-4.235213	-0.902014
6	-5.661740	4.268487	0.201435
6	-5.524478	4.144322	-1.170813
6	-5.386814	-3.878339	2.079113
6	-5.260252	-3.069466	3.199289
6	-5.236048	2.281670	-3.498532
6	-5.110716	0.957669	-3.997993
6	-5.014254	-0.282163	4.280803
6	-4.908654	1.120859	4.063984
6	-4.836565	-1.883307	-3.679707
6	-4.691758	-3.062932	-2.830480
6	-4.664648	3.450450	2.400749
6	-4.528349	4.070952	1.080606
6	-4.395321	-4.270562	-0.237564

6	-4.254158	-4.134539	1.219926
6	-4.243371	3.843941	-1.769984
6	-4.110713	2.968572	-2.960526
6	-3.991064	-2.485846	3.560057
6	-3.878909	-1.127706	4.154715
6	-3.801401	0.351439	-4.074072
6	-3.668204	-1.088842	-3.942632
6	-3.608257	1.703714	3.833625
6	-3.490744	2.897047	3.013668
6	-3.381235	-3.423098	-2.354634
6	-3.235117	-4.056145	-1.054443
6	-3.221684	4.153483	0.482363
6	-3.081138	4.061353	-0.960831
6	-2.951502	-3.868281	1.766540
6	-2.820158	-3.057448	2.962961
6	-2.788452	2.478573	-3.302998
6	-2.638024	1.184757	-3.914458
6	-2.564383	-0.513121	4.208514
6	-2.433582	0.914768	4.104583
6	-2.345497	-1.651473	-3.744656
6	-2.201621	-2.850744	-2.978861
6	-2.171545	3.305254	2.562731
6	-2.037285	3.971613	1.305032
6	-1.907468	-4.160405	-0.466452
6	-1.765827	-4.103489	0.955243
6	-1.748935	3.869042	-1.528093
6	-1.605732	3.111446	-2.735489
6	-1.493143	-2.585187	3.353188
6	-1.368762	-1.325637	4.028572
6	-1.310990	0.594721	-4.046325
6	-1.169754	-0.837138	-4.007306
6	-1.114111	1.513375	3.935448
6	-0.989251	2.744009	3.193952
6	-0.876829	-3.273114	-2.552593
6	-0.732469	-3.974741	-1.297618
6	-0.716895	4.140310	0.723418
6	-0.577599	4.127349	-0.720325
6	-0.447739	-3.932984	1.536317
6	-0.316424	-3.190904	2.778524
6	-0.287742	2.680628	-3.155878
6	-0.143520	1.418749	-3.861085
6	-0.062410	-0.724302	4.181391
6	0.062417	0.725407	4.181201
6	0.143524	-1.419771	-3.860711
6	0.287742	-2.681466	-3.155173
6	0.316424	3.191640	2.777683
6	0.447735	3.933393	1.535278
6	0.577592	-4.127544	-0.719237
6	0.716889	-4.140122	0.724510
6	0.732464	3.974398	-1.298666
6	0.876827	3.272440	-2.553455
6	0.989253	-2.743165	3.194672
6	1.114117	-1.512334	3.935841
6	1.169758	0.836078	-4.007520
6	1.310994	-0.595793	-4.046164
6	1.368768	1.326702	4.028216
6	1.493145	2.586076	3.352502
6	1.605731	-3.112176	-2.734668
6	1.748930	-3.869455	-1.527073
6	1.765821	4.103750	0.954160
6	1.907462	4.160291	-0.467550
6	2.037281	-3.971276	1.306078
6	2.171545	-3.304580	2.563598
6	2.201620	2.849957	-2.979607
6	2.345500	1.650481	-3.745079
6	2.433589	-0.913683	4.104811
6	2.564390	0.514234	4.208367
6	2.638028	-1.185793	-3.914133
6	2.788453	-2.479452	-3.302341
6	2.820158	3.058238	2.962150

6	2.951497	3.868763	1.765519
6	3.081132	-4.061625	-0.959762
6	3.221678	-4.153371	0.483457
6	3.235111	4.055879	-1.055513
6	3.381232	3.422482	-2.355532
6	3.490746	-2.896254	3.014423
6	3.608263	-1.702701	3.834058
6	3.668210	1.087798	-3.942899
6	3.801406	-0.352518	-4.073958
6	3.878916	1.128805	4.154398
6	3.991067	2.486795	3.559392
6	4.110712	-2.969366	-2.959739
6	4.243366	-3.844429	-1.768972
6	4.254152	4.134883	1.218835
6	4.395314	4.270522	-0.238692
6	4.528343	-4.070687	1.081677
6	4.664647	-3.449825	2.401649
6	4.691758	3.062194	-2.831280
6	4.836569	1.882334	-3.680182
6	4.908661	-1.119784	4.064255
6	5.014262	0.283296	4.280699
6	5.110721	-0.958729	-3.997718
6	5.236049	-2.282604	-3.497921
6	5.260253	3.070327	3.198472
6	5.386809	3.878916	2.078090
6	5.524473	-4.144662	-1.169724
6	5.661734	-4.268466	0.202558
6	5.683213	4.235003	-0.903133
6	5.824373	3.668650	-2.155612
6	5.956631	-3.045436	2.943637
6	6.075663	-1.940113	3.755363
6	6.134865	1.279742	-3.968468
6	6.267848	-0.077965	-4.141190
1	-7.263379	0.527799	-4.255146
1	-7.031029	-1.914402	-3.949657
1	-7.067644	1.587809	4.069025
1	-6.860738	3.575087	2.614491
1	-6.829085	-3.555249	-2.581357
1	-6.578519	-4.559902	-0.356155
1	-6.665857	4.376351	0.630857
1	-6.423893	4.155837	-1.800072
1	-6.387407	-4.202204	1.765587
1	-6.164879	-2.772849	3.745820
1	-6.247253	2.665342	-3.313209
1	-6.019963	-0.720603	4.306113
1	6.019974	0.721741	4.305883
1	6.247250	-2.666235	-3.312510
1	6.164881	2.773853	3.745078
1	6.387393	4.202705	1.764483
1	6.423885	-4.156348	-1.798982
1	6.665847	-4.376223	0.632008
1	6.578512	4.559846	-0.357362
1	6.829082	3.554598	-2.582293
1	6.860739	-3.574398	2.615409
1	7.067654	-1.586721	4.069397
1	7.031035	1.913353	-3.950125
1	7.263385	-0.528926	-4.254971

Nanotube (7,5) u05v02
B3LYP/STO-3G Energy: -4682.245478

6	-6.632703	-3.584016	-1.174573
6	-6.520437	-3.772336	0.182259
6	-5.869529	4.487419	-0.949062
6	-5.778303	3.979537	-2.224467
6	-6.150162	-2.656659	2.958172
6	-5.942047	-1.605134	3.828992
6	-5.640386	1.629164	-4.109543

6	-5.598815	0.265720	-4.342100
6	-5.443264	1.339666	4.252097
6	-5.222497	2.616112	3.758068
6	-5.509728	-2.474042	-3.135360
6	-5.447944	-3.299988	-1.982915
6	-4.831834	4.349661	1.341969
6	-4.705189	4.488918	-0.067405
6	-5.219910	-3.736146	0.846814
6	-5.048609	-3.230274	2.204963
6	-4.516137	3.465451	-2.745621
6	-4.454394	2.345519	-3.684808
6	-4.614075	-1.062771	4.044183
6	-4.375065	0.365975	4.290246
6	-4.367196	-0.480302	-4.199294
6	-4.334485	-1.859107	-3.657270
6	-3.915904	3.024105	3.297786
6	-3.728453	3.931983	2.137368
6	-4.160209	-3.618910	-1.408363
6	-4.052485	-3.867705	0.018586
6	-3.408250	4.320631	-0.680627
6	-3.316678	3.828845	-2.044112
6	-3.718934	-2.955286	2.685175
6	-3.504413	-1.875902	3.635139
6	-3.188837	1.697842	-3.914608
6	-3.148271	0.273220	-4.198362
6	-3.033245	0.870585	4.187879
6	-2.802339	2.222672	3.711994
6	-3.049951	-2.407714	-3.264627
6	-2.970368	-3.335230	-2.166712
6	-2.398408	4.044906	1.567140
6	-2.238711	4.295130	0.159681
6	-2.733710	-3.910671	0.621378
6	-2.569036	-3.489681	1.978296
6	-2.022297	3.404716	-2.546748
6	-1.956810	2.357839	-3.518586
6	-2.144920	-1.428319	3.898444
6	-1.909835	-0.054513	4.214926
6	-1.862825	-0.417303	-4.152189
6	-1.818293	-1.783197	-3.726456
6	-1.441311	2.625907	3.366591
6	-1.239270	3.581517	2.318442
6	-1.668578	-3.702617	-1.620964
6	-1.558301	-4.036370	-0.226119
6	-0.919602	4.184114	-0.452445
6	-0.814246	3.778246	-1.830096
6	-1.229236	-3.277992	2.504847
6	-1.021090	-2.262277	3.510171
6	-0.674474	1.746326	-3.826803
6	-0.632887	0.345839	-4.188916
6	-0.551823	0.457799	4.213664
6	-0.319216	1.835622	3.820452
6	-0.539936	-2.391107	-3.409736
6	-0.472261	-3.398048	-2.365407
6	0.091961	3.785688	1.785573
6	0.251743	4.133386	0.383928
6	-0.251740	-4.133490	0.382835
6	-0.091960	-3.786161	1.784573
6	0.472263	3.398673	-2.364508
6	0.539936	2.392010	-3.409105
6	0.319212	-1.836633	3.819968
6	0.551817	-0.458914	4.213543
6	0.632885	-0.344730	-4.189008
6	0.674473	-1.745312	-3.827266
6	1.021087	2.261347	3.510772
6	1.229236	3.277327	2.505715
6	0.814250	-3.777760	-1.831095
6	0.919606	-4.183991	-0.453552
6	1.558305	4.036425	-0.225050
6	1.668581	3.703042	-1.619984
6	1.239271	-3.582130	2.317495

6	1.441308	-2.626798	3.365899
6	1.818292	1.784183	-3.725987
6	1.862823	0.418403	-4.152084
6	1.909830	0.053397	4.214948
6	2.144917	1.427287	3.898828
6	1.956811	-2.356905	-3.519211
6	2.022300	-3.404037	-2.547649
6	2.569037	3.489153	1.979222
6	2.733712	3.910498	0.622414
6	2.238716	-4.295166	0.158546
6	2.398410	-4.045316	1.566072
6	2.970369	3.335800	-2.165830
6	3.049951	2.408576	-3.263994
6	2.802334	-2.223653	3.711413
6	3.033239	-0.871695	4.187658
6	3.148269	-0.272108	-4.198443
6	3.188837	-1.696804	-3.915063
6	3.504409	1.874938	3.635642
6	3.718934	2.954569	2.685960
6	3.316682	-3.828295	-2.045124
6	3.408255	-4.320441	-0.681769
6	4.052487	3.867687	0.019611
6	4.160211	3.619272	-1.407403
6	3.728455	-3.932540	2.136331
6	3.915903	-3.024973	3.296993
6	4.334484	1.860073	-3.656785
6	4.367193	0.481416	-4.199178
6	4.375059	-0.367112	4.290163
6	4.614070	1.061697	4.044476
6	4.454394	-2.344538	-3.685434
6	4.516140	-3.464714	-2.746536
6	5.048611	3.229679	2.205818
6	5.219913	3.735905	0.847803
6	4.705195	-4.488882	-0.068590
6	4.831839	-4.349999	1.340821
6	5.447945	3.300502	-1.982043
6	5.509727	2.474872	-3.134713
6	5.222491	-2.617106	3.757394
6	5.443257	-1.340793	4.251764
6	5.598812	-0.264567	-4.342185
6	5.640385	-1.628072	-4.109989
6	5.942043	1.604112	3.829425
6	6.150162	2.655862	2.958877
6	5.778308	-3.978930	-2.225517
6	5.869535	-4.487145	-0.950246
6	6.520439	3.772269	0.183257
6	6.632704	3.584313	-1.173625
1	-7.622720	-3.512060	-1.646130
1	-7.427820	-3.856689	0.794255
1	-6.845977	4.774250	-0.534187
1	-6.688436	3.866586	-2.827743
1	-7.177226	-2.970599	2.731506
1	-6.807340	-1.101144	4.278731
1	-6.610260	2.143021	-4.109121
1	-6.537579	-0.274439	-4.521132
1	-6.470361	1.024185	4.476487
1	-6.080779	3.282800	3.603256
1	-6.497223	-2.127565	-3.465538
1	-5.844070	4.336999	1.765762
1	5.844077	-4.337434	1.764615
1	6.497219	2.128497	-3.464998
1	6.080776	-3.283751	3.602406
1	6.470355	-1.025375	4.476249
1	6.537577	0.275641	-4.521079
1	6.610259	-2.141930	-4.109706
1	6.807335	1.100000	4.279029
1	7.177226	2.969852	2.732286
1	6.688441	-3.865818	-2.828761
1	6.845986	-4.774082	-0.535448
1	7.427823	3.856456	0.795275

1 7.622722 3.512483 -1.645202

Nanotube (7,5) u05v03
B3LYP/STO-3G Energy: -4757.540481

6	6.555999	-3.539303	1.940489
6	6.380553	-4.059388	0.681034
6	6.258882	4.235347	-0.345966
6	6.183604	4.077570	1.018010
6	5.971821	-3.669533	-2.280035
6	5.794953	-2.865995	-3.388287
6	5.978049	2.304714	3.449094
6	5.866758	1.053818	4.028138
6	5.459677	-0.101945	-4.549959
6	5.334160	1.269580	-4.399440
6	5.575378	-1.892440	3.572676
6	5.421592	-2.978609	2.674686
6	5.134104	3.585338	-2.503568
6	5.065561	4.086265	-1.176219
6	5.059279	-4.104934	0.057407
6	4.866748	-3.952201	-1.379179
6	4.912319	3.795974	1.678507
6	4.819826	2.962661	2.875618
6	4.494442	-2.306371	-3.708212
6	4.333275	-0.978979	-4.312659
6	4.588885	0.377473	4.109003
6	4.456841	-1.088135	3.945092
6	4.070685	1.869655	-4.035295
6	3.979173	3.052824	-3.144960
6	4.095647	-3.349025	2.230741
6	3.918166	-3.943731	0.918038
6	3.782948	4.165688	-0.515045
6	3.711496	4.045162	0.930590
6	3.538043	-3.718845	-1.885513
6	3.353293	-2.908923	-3.078521
6	3.528135	2.480243	3.291555
6	3.416211	1.183239	3.938127
6	3.028373	-0.375714	-4.321673
6	2.896690	1.066133	-4.209822
6	3.129936	-1.635081	3.738629
6	2.954912	-2.806067	2.918940
6	2.679756	3.396508	-2.597974
6	2.585433	4.005021	-1.297568
6	2.577449	-4.048538	0.375803
6	2.386520	-3.973862	-1.040197
6	2.413914	3.848055	1.550484
6	2.322970	3.092879	2.761145
6	2.015350	-2.453048	-3.421314
6	1.851551	-1.197184	-4.083777
6	2.092956	0.589432	4.099948
6	1.954435	-0.833253	4.048203
6	1.576351	1.635254	-3.955149
6	1.469428	2.836099	-3.183673
6	1.614505	-3.214235	2.515291
6	1.430466	-3.877277	1.254383
6	1.284382	4.138364	-0.651385
6	1.204363	4.102805	0.784974
6	1.042764	-3.808092	-1.573144
6	0.858368	-3.076150	-2.801715
6	1.018670	2.665513	3.242419
6	0.909758	1.414558	3.959837
6	0.527029	-0.610675	-4.191717
6	0.391991	0.831191	-4.169174
6	0.631704	-1.418789	3.930740
6	0.465785	-2.654212	3.187508
6	0.170996	3.257764	-2.695316
6	0.082624	3.956207	-1.424862
6	0.095608	-4.036181	0.719776

6	-0.095623	-4.036340	-0.718898
6	-0.082643	3.956522	1.424006
6	-0.171001	3.258359	2.694614
6	-0.465780	-2.654915	-3.186938
6	-0.631687	-1.419654	-3.930442
6	-0.391970	0.832107	4.169004
6	-0.527008	-0.609755	4.191858
6	-0.909742	1.413685	-3.960152
6	-1.018667	2.664792	-3.243001
6	-0.858368	-3.075525	2.802385
6	-1.042776	-3.807729	1.573972
6	-1.204385	4.102610	-0.785862
6	-1.284405	4.138486	0.650488
6	-1.430478	-3.877538	-1.253542
6	-1.614507	-3.214781	-2.514601
6	-1.469427	2.836794	3.183073
6	-1.576334	1.636122	3.954820
6	-1.954416	-0.834145	-4.048053
6	-2.092937	0.588529	-4.100107
6	-1.851532	-1.196286	4.084062
6	-2.015342	-2.452286	3.421859
6	-2.322973	3.092251	-2.761824
6	-2.413932	3.847678	-1.551319
6	-2.386535	-3.973597	1.041061
6	-2.577465	-4.048584	-0.374923
6	-2.585454	4.005267	1.296702
6	-2.679764	3.397057	2.597251
6	-2.954909	-2.806699	-2.918353
6	-3.129921	-1.635903	-3.738316
6	-2.896668	1.067056	4.209641
6	-3.028349	-0.374766	4.321805
6	-3.416194	1.182369	-3.938431
6	-3.528130	2.479503	-3.292121
6	-3.353291	-2.908222	3.079167
6	-3.538054	-3.718385	1.886324
6	-3.711518	4.044894	-0.931467
6	-3.782972	4.165733	0.514142
6	-3.918180	-3.943882	-0.917184
6	-4.095652	-3.349485	-2.230029
6	-3.979174	3.053489	3.144327
6	-4.070668	1.870535	4.034951
6	-4.456824	-1.089004	-3.944923
6	-4.588866	0.376567	-4.109160
6	-4.333252	-0.978029	4.312937
6	-4.494431	-2.305536	3.708748
6	-4.819828	2.961994	-2.876289
6	-4.912336	3.795533	-1.679337
6	-4.866763	-3.951826	1.380037
6	-5.059295	-4.104869	-0.056515
6	-5.065584	4.086434	1.175335
6	-5.134116	3.585822	2.502804
6	-5.421592	-2.979166	-2.674070
6	-5.575366	-1.893217	-3.572329
6	-5.334136	1.270546	4.399267
6	-5.459649	-0.100947	4.550088
6	-5.866741	1.052927	-4.028462
6	-5.978042	2.303934	-3.449660
6	-5.794949	-2.865204	3.388933
6	-5.971832	-3.668954	2.280835
6	-6.183625	4.077235	-1.018895
6	-6.258907	4.235299	0.345048
6	-6.380569	-4.059443	-0.680153
6	-6.556007	-3.539664	-1.939737
1	7.565591	-3.417080	2.356743
1	7.256651	-4.359368	0.091700
1	7.234551	4.343799	-0.839853
1	7.105937	4.065483	1.613039
1	6.985272	-3.986610	-2.002750
1	6.670701	-2.557004	-3.973512
1	6.974739	2.738538	3.297619

1	6.778220	0.518764	4.324663
1	6.456628	-0.533641	-4.706258
1	6.235418	1.894910	-4.440347
1	6.592926	-1.538085	3.781255
1	6.127862	3.398700	-2.930324
1	-6.127879	3.399256	2.929598
1	-6.592914	-1.538907	-3.780997
1	-6.235390	1.895886	4.440064
1	-6.456591	-0.532609	4.706509
1	-6.778195	0.517816	-4.324907
1	-6.974733	2.737791	-3.298289
1	-6.670693	-2.556085	3.974098
1	-6.985294	-3.986068	2.003607
1	-7.105960	4.065001	-1.613921
1	-7.234581	4.343830	0.838910
1	-7.256673	-4.359265	-0.090745
1	-7.565595	-3.417527	-2.356019

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B3LYP/STO-3G Energy: -4832.835097

6	6.699862	2.636001	-2.992093
6	6.606167	3.466500	-1.902183
6	6.202352	-4.277687	1.222487
6	6.064876	-4.466022	-0.132188
6	6.323313	3.861223	1.073269
6	6.167383	3.375180	2.354913
6	5.809393	-3.360271	-2.926391
6	5.720885	-2.295088	-3.802742
6	5.779815	1.019472	4.199077
6	5.594150	-0.335980	4.412365
6	5.574577	0.681004	-4.109950
6	5.509247	1.965754	-3.517042
6	5.212560	-3.045553	3.183523
6	5.058622	-3.861722	2.033030
6	5.318624	3.736070	-1.263196
6	5.188336	3.961012	0.169282
6	4.773793	-4.293970	-0.793748
6	4.655069	-3.787492	-2.157631
6	4.861567	2.980173	2.853388
6	4.677557	1.861907	3.783519
6	4.469034	-1.594372	-4.005854
6	4.405846	-0.132753	-4.222068
6	4.291222	-0.945685	4.261944
6	4.110752	-2.310386	3.711869
6	4.221932	2.506756	-3.136740
6	4.131753	3.422643	-2.014357
6	3.741716	-4.042551	1.463863
6	3.602327	-4.285732	0.039056
6	3.876337	3.931406	0.765827
6	3.716354	3.459945	2.131951
6	3.364308	-3.359157	-2.633585
6	3.273595	-2.266669	-3.588233
6	3.351996	1.347482	3.995928
6	3.159206	-0.066531	4.266738
6	3.114403	0.518208	-4.118266
6	3.028172	1.868157	-3.622996
6	2.774500	-2.718643	3.323401
6	2.592228	-3.632308	2.226169
6	2.824216	3.730470	-1.469485
6	2.697839	4.023273	-0.074426
6	2.284692	-4.183643	-0.559718
6	2.163925	-3.751966	-1.917934
6	2.379578	3.172680	2.626998
6	2.198330	2.137401	3.595264
6	1.970471	-1.665182	-3.848148
6	1.893194	-0.272779	-4.165274
6	1.807482	-0.615343	4.216785

6	1.616824	-1.966780	3.789422
6	1.727255	2.435449	-3.290345
6	1.630935	3.402852	-2.234774
6	1.256733	-3.859764	1.685824
6	1.105936	-4.177115	0.292419
6	1.374621	4.063639	0.530843
6	1.219424	3.674742	1.909535
6	0.855628	-3.388538	-2.439673
6	0.762139	-2.361021	-3.449853
6	0.857645	1.664639	3.897957
6	0.665609	0.275632	4.256910
6	0.602512	0.393330	-4.157452
6	0.524209	1.783130	-3.756661
6	0.279890	-2.436085	3.478061
6	0.101077	-3.431421	2.436663
6	0.329280	3.760620	-1.710815
6	0.206942	4.129192	-0.312537
6	-0.206933	-4.129212	-0.312278
6	-0.329274	-3.760730	-1.710580
6	-0.101076	3.431578	2.436448
6	-0.279895	2.436307	3.477908
6	-0.524213	-1.783369	-3.756549
6	-0.602519	-0.393592	-4.157424
6	-0.665621	-0.275362	4.256922
6	-0.857653	-1.664392	3.898056
6	-0.762141	2.360803	-3.449997
6	-0.855625	3.388386	-2.439884
6	-1.219420	-3.674626	1.909764
6	-1.374613	-4.063614	0.531097
6	-1.105927	4.177144	0.292157
6	-1.256727	3.859881	1.685581
6	-1.630931	-3.403002	-2.234560
6	-1.727256	-2.435661	-3.290189
6	-1.616832	1.967021	3.789289
6	-1.807493	0.615610	4.216731
6	-1.893200	0.272515	-4.165278
6	-1.970476	1.664939	-3.848240
6	-2.198336	-2.137175	3.595387
6	-2.379577	-3.172521	2.627192
6	-2.163919	3.751856	-1.918168
6	-2.284682	4.183625	-0.559982
6	-2.697831	-4.023297	-0.074176
6	-2.824210	-3.730580	-1.469252
6	-2.592225	3.632463	2.225938
6	-2.774504	2.718860	3.323219
6	-3.028175	-1.868390	-3.622866
6	-3.114409	-0.518469	-4.118213
6	-3.159218	0.066802	4.266707
6	-3.352005	-1.347229	3.995989
6	-3.273598	2.266443	-3.588357
6	-3.364306	3.359000	-2.633788
6	-3.716351	-3.459827	2.132163
6	-3.876330	-3.931385	0.766072
6	-3.602316	4.285764	0.038786
6	-3.741708	4.042672	1.463608
6	-4.131748	-3.422792	-2.014143
6	-4.221932	-2.506966	-3.136574
6	-4.110759	2.310628	3.711703
6	-4.291234	0.945956	4.261850
6	-4.405854	0.132485	-4.222046
6	-4.469040	1.594118	-4.005924
6	-4.677565	-1.861671	3.783610
6	-4.861567	-2.980010	2.853564
6	-4.655064	3.787376	-2.157864
6	-4.773782	4.293958	-0.794018
6	-5.188328	-3.961040	0.169527
6	-5.318618	-3.736185	-1.262964
6	-5.058616	3.861885	2.032784
6	-5.212562	3.045774	3.183317
6	-5.509249	-1.965987	-3.516900

6	-5.574584	-0.681265	-4.109870
6	-5.594163	0.336259	4.412294
6	-5.779826	-1.019207	4.199096
6	-5.720889	2.294847	-3.802854
6	-5.809391	3.360098	-2.926584
6	-6.167380	-3.375065	2.355117
6	-6.323306	-3.861200	1.073508
6	-6.064864	4.466069	-0.132470
6	-6.202342	4.277818	1.222218
6	-6.606162	-3.466656	-1.901966
6	-6.699861	-2.636212	-2.991915
1	7.682391	2.361011	-3.400028
1	7.520694	3.861563	-1.441270
1	7.196129	-4.309231	1.690234
1	6.955424	-4.653774	-0.745816
1	7.333883	4.048413	0.688551
1	7.056448	3.183089	2.969347
1	6.793022	-3.795277	-2.708347
1	6.636928	-1.903697	-4.263895
1	6.798641	1.427388	4.204177
1	6.470752	-0.974369	4.582610
1	6.565040	0.231817	-4.257182
1	6.232525	-2.806490	3.510790
1	-6.232527	2.806737	3.510596
1	-6.565052	-0.232083	-4.257114
1	-6.470768	0.974659	4.582484
1	-6.798655	-1.427121	4.204205
1	-6.636936	1.903419	-4.263968
1	-6.793017	3.795121	-2.708568
1	-7.056447	-3.182938	2.969539
1	-7.333878	-4.048420	0.688799
1	-6.955409	4.653795	-0.746110
1	-7.196116	4.309405	1.689963
1	-7.520687	-3.861700	-1.441033
1	-7.682391	-2.361246	-3.399863

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B3LYP/STO-3G Energy: -4908.129191

6	-6.875134	-2.009422	-3.328638
6	-6.704719	-3.087321	-2.495579
6	-6.359976	3.609181	2.502919
6	-6.295690	4.142826	1.238266
6	-6.259418	-4.218895	0.264150
6	-6.050304	-4.069776	1.618911
6	-6.147078	3.799692	-1.754706
6	-6.071735	2.998856	-2.877637
6	-5.632908	-2.251805	3.989647
6	-5.475468	-0.991030	4.538112
6	-5.859428	0.209471	-3.946847
6	-5.730178	-1.179817	-3.710631
6	-5.237006	1.956790	4.036546
6	-5.165164	3.046049	3.131905
6	-5.379121	-3.461838	-2.001907
6	-5.169917	-4.039708	-0.683970
6	-5.034144	4.197883	0.502217
6	-4.968144	4.061248	-0.947937
6	-4.730909	-3.762066	2.145203
6	-4.530003	-2.912573	3.320984
6	-4.811315	2.422342	-3.303858
6	-4.718790	1.070163	-3.892224
6	-4.199782	-0.309023	4.493640
6	-4.087571	1.156139	4.311031
6	-4.410909	-1.750984	-3.538723
6	-4.240109	-2.921503	-2.697953
6	-3.883648	3.422611	2.576265
6	-3.822490	4.027003	1.257824
6	-3.829611	-4.114006	-0.156662

6	-3.611489	-3.998249	1.276205
6	-3.690316	3.821024	-1.570001
6	-3.616011	3.012353	-2.776143
6	-3.209797	-2.415518	3.600994
6	-3.043773	-1.112260	4.221101
6	-3.407266	0.465296	-4.013971
6	-3.260600	-0.962972	-3.891382
6	-2.785356	1.706984	3.989347
6	-2.685903	2.880140	3.160478
6	-2.899905	-3.310077	-2.308595
6	-2.694651	-3.945460	-1.042490
6	-2.534331	4.135252	0.600169
6	-2.468474	4.066537	-0.827049
6	-2.259695	-3.791618	1.768958
6	-2.057363	-3.027575	2.959941
6	-2.311380	2.547738	-3.232952
6	-2.211504	1.288146	-3.901542
6	-1.713786	-0.513639	4.257783
6	-1.584135	0.908848	4.193623
6	-1.930218	-1.546340	-3.771814
6	-1.755650	-2.749718	-3.012074
6	-1.386925	3.294283	2.643606
6	-1.315026	3.960953	1.374414
6	-1.341429	-4.087971	-0.525096
6	-1.125141	-4.050642	0.896792
6	-1.176817	3.898331	-1.476303
6	-1.103862	3.165438	-2.716944
6	-0.716461	-2.589834	3.312106
6	-0.545647	-1.336118	4.010453
6	-0.903577	0.693043	-4.118639
6	-0.768340	-0.748426	-4.100068
6	-0.278229	1.499636	3.962088
6	-0.181574	2.736139	3.212754
6	-0.419756	-3.183004	-2.656290
6	-0.216047	-3.895791	-1.409307
6	-0.031650	4.122928	0.724796
6	0.031648	4.122882	-0.725055
6	0.216044	-3.895699	1.409552
6	0.419755	-3.182832	2.656489
6	0.181575	2.735932	-3.212923
6	0.278231	1.499382	-3.962180
6	0.768343	-0.748164	4.100112
6	0.903580	0.693306	4.118594
6	0.545649	-1.336375	-4.010368
6	0.716462	-2.590048	-3.311944
6	1.103862	3.165614	2.716746
6	1.176816	3.898428	1.476059
6	1.125138	-4.050703	-0.896537
6	1.341426	-4.087939	0.525353
6	1.315024	3.960866	-1.374663
6	1.386925	3.294114	-2.643811
6	1.755650	-2.749525	3.012244
6	1.930220	-1.546099	3.771907
6	1.584138	0.908580	-4.193675
6	1.713789	-0.513911	-4.257747
6	2.211506	1.288396	3.901458
6	2.311381	2.547947	3.232791
6	2.057363	-3.027768	-2.959750
6	2.259692	-3.791737	-1.768720
6	2.468472	4.066595	0.826794
6	2.534329	4.135219	-0.600429
6	2.694649	-3.945398	1.042737
6	2.899904	-3.309931	2.308800
6	2.685904	2.879939	-3.160655
6	2.785358	1.706728	-3.989448
6	3.260602	-0.962724	3.891435
6	3.407268	0.465553	4.013935
6	3.043775	-1.112531	-4.221026
6	3.209797	-2.415751	-3.600840
6	3.616012	3.012535	2.775953

6	3.690315	3.821133	1.569762
6	3.611486	-3.998340	-1.275953
6	3.829607	-4.114004	0.156920
6	3.822489	4.026929	-1.258076
6	3.883648	3.422449	-2.576477
6	4.240108	-2.921332	2.698132
6	4.410910	-1.750757	3.538823
6	4.087574	1.155863	-4.311093
6	4.199786	-0.309309	-4.493610
6	4.718793	1.070411	3.892147
6	4.811316	2.422556	3.303702
6	4.530003	-2.912791	-3.320798
6	4.730906	-3.762213	-2.144966
6	4.968143	4.061319	0.947682
6	5.034142	4.197861	-0.502480
6	5.169914	-4.039674	0.684224
6	5.379120	-3.461715	2.002120
6	5.165165	3.045852	-3.132090
6	5.237008	1.956532	-4.036658
6	5.730180	-1.179581	3.710692
6	5.859430	0.209723	3.946819
6	5.475472	-0.991320	-4.538037
6	5.632910	-2.252062	-3.989496
6	6.071736	2.999046	2.877446
6	6.147077	3.799815	1.754468
6	6.050300	-4.069896	-1.618656
6	6.259414	-4.218929	-0.263885
6	6.295688	4.142758	-1.238526
6	6.359976	3.609028	-2.503142
6	6.704718	-3.087165	2.495766
6	6.875134	-2.009210	3.328751
1	-7.883724	-1.677681	-3.611663
1	-7.583705	-3.623763	-2.115419
1	-7.329501	3.480131	3.003643
1	-7.220516	4.445652	0.730451
1	-7.282862	-4.343038	-0.111992
1	-6.910658	-4.077518	2.300513
1	-7.130197	4.127515	-1.393681
1	-6.997339	2.704385	-3.389003
1	-6.637314	-2.690762	3.935445
1	-6.359165	-0.455420	4.908458
1	-6.867525	0.643157	-3.932787
1	-6.231410	1.598896	4.332517
1	6.231415	1.598617	-4.332603
1	6.867527	0.643408	3.932731
1	6.359169	-0.455731	-4.908413
1	6.637316	-2.691016	-3.935266
1	6.997340	2.704608	3.388830
1	7.130194	4.127619	1.393425
1	6.910654	-4.077687	-2.300258
1	7.282858	-4.343054	0.112265
1	7.220513	4.445621	-0.730730
1	7.329504	3.479942	-3.003856
1	7.583704	-3.623633	2.115641
1	7.883726	-1.677450	3.611752

Nanotube (7,5) u05v06
B3LYP/STO-3G Energy: -4983.423049

6	-6.805272	-0.954207	-4.023434
6	-6.693490	-2.213305	-3.488399
6	-6.558623	2.976242	3.070833
6	-6.420984	3.814404	1.991396
6	-6.414272	-4.023445	-1.091743
6	-6.277768	-4.229272	0.264365
6	-6.110023	4.243323	-0.978893
6	-5.978688	3.752555	-2.262650
6	-5.969267	-3.085870	3.039114

6	-5.828264	-2.010993	3.897894
6	-5.733096	1.323057	-3.996043
6	-5.631780	-0.082210	-4.118068
6	-5.534801	0.960371	4.180357
6	-5.404293	2.242490	3.592621
6	-5.401492	-2.734748	-3.039986
6	-5.272086	-3.635341	-1.907201
6	-5.119989	4.027921	1.358550
6	-4.975208	4.264102	-0.071306
6	-4.985035	-4.098033	0.917266
6	-4.838436	-3.580541	2.277732
6	-4.700871	3.272835	-2.755222
6	-4.588029	2.113658	-3.661874
6	-4.544162	-1.369442	4.090986
6	-4.408015	0.089427	4.296345
6	-4.329842	-0.710939	-4.030992
6	-4.219018	-2.062069	-3.515062
6	-4.090603	2.721353	3.219214
6	-3.952493	3.643786	2.107009
6	-3.963277	-3.877235	-1.350522
6	-3.822363	-4.135398	0.073160
6	-3.666365	4.163293	-0.667857
6	-3.531367	3.683842	-2.033990
6	-3.529649	-3.202957	2.740367
6	-3.383532	-2.103758	3.679616
6	-3.277669	1.528080	-3.865144
6	-3.152984	0.112603	-4.107479
6	-3.085932	0.674476	4.192899
6	-2.931368	2.019843	3.702342
6	-2.907230	-2.572480	-3.173561
6	-2.779825	-3.517928	-2.105904
6	-2.630258	3.890510	1.566877
6	-2.486370	4.187314	0.174780
6	-2.497682	-4.094286	0.668799
6	-2.351604	-3.659907	2.022690
6	-2.207974	3.318550	-2.523768
6	-2.082547	2.265104	-3.482168
6	-2.051802	-1.564415	3.931501
6	-1.904819	-0.177019	4.241003
6	-1.838368	-0.514700	-4.073507
6	-1.719427	-1.878094	-3.647394
6	-1.602775	2.523945	3.375855
6	-1.456264	3.494920	2.330682
6	-1.459187	-3.822807	-1.575565
6	-1.320351	-4.152550	-0.183688
6	-1.162106	4.161630	-0.428835
6	-1.025711	3.760273	-1.805622
6	-1.026086	-3.355930	2.539143
6	-0.879597	-2.324100	3.538721
6	-0.769966	1.711169	-3.771045
6	-0.650602	0.312601	-4.118352
6	-0.581952	0.423357	4.233824
6	-0.433646	1.809098	3.839198
6	-0.409699	-2.424533	-3.350367
6	-0.283704	-3.440180	-2.325280
6	-0.137428	3.793544	1.812214
6	0.006179	4.166585	0.417551
6	-0.006179	-4.166563	0.417765
6	0.137428	-3.793450	1.812409
6	0.283704	3.440059	-2.325456
6	0.409700	2.424359	-3.350491
6	0.433645	-1.808899	3.839291
6	0.581951	-0.423138	4.233847
6	0.650603	-0.312814	-4.118336
6	0.769966	-1.711365	-3.770958
6	0.879597	2.324283	3.538602
6	1.026085	3.356062	2.538971
6	1.025710	-3.760367	-1.805430
6	1.162106	-4.161652	-0.428620
6	1.320350	4.152541	-0.183901

6	1.459187	3.822726	-1.575761
6	1.456264	-3.494798	2.330862
6	1.602774	-2.523769	3.375984
6	1.719428	1.877905	-3.647489
6	1.838368	0.514489	-4.073533
6	1.904818	0.177238	4.240994
6	2.051801	1.564618	3.931421
6	2.082548	-2.265284	-3.482051
6	2.207974	-3.318681	-2.523597
6	2.351603	3.660013	2.022503
6	2.497682	4.094321	0.668589
6	2.486370	-4.187304	0.174995
6	2.630258	-3.890428	1.567077
6	2.779825	3.517818	-2.106084
6	2.907230	2.572316	-3.173692
6	2.931368	-2.019650	3.702445
6	3.085933	-0.674259	4.192933
6	3.152985	-0.112816	-4.107472
6	3.277670	-1.528280	-3.865065
6	3.383531	2.103949	3.679509
6	3.529648	3.203099	2.740204
6	3.531367	-3.683949	-2.033801
6	3.666365	-4.163328	-0.667643
6	3.822364	4.135402	0.072948
6	3.963277	3.877165	-1.350720
6	3.952493	-3.643676	2.107196
6	4.090603	-2.721185	3.219353
6	4.219019	2.061886	-3.515167
6	4.329843	0.710730	-4.031027
6	4.408015	-0.089204	4.296349
6	4.544161	1.369656	4.090917
6	4.588030	-2.113848	-3.661765
6	4.700872	-3.272980	-2.755054
6	4.838435	3.580660	2.277551
6	4.985034	4.098082	0.917057
6	4.975208	-4.264109	-0.071088
6	5.119988	-4.027852	1.358757
6	5.272086	3.635243	-1.907386
6	5.401493	2.734591	-3.040126
6	5.404293	-2.242302	3.592733
6	5.534801	-0.960153	4.180403
6	5.631781	0.081996	-4.118072
6	5.733097	-1.323265	-3.995974
6	5.828262	2.011199	3.897794
6	5.969265	3.086031	3.038961
6	5.978688	-3.752678	-2.262459
6	6.110021	-4.243382	-0.978677
6	6.277768	4.229285	0.264150
6	6.414273	4.023388	-1.091948
6	6.420984	-3.814300	1.991590
6	6.558624	-2.976080	3.070983
6	6.693490	2.213125	-3.488511
6	6.805273	0.953998	-4.023482
1	-7.792663	-0.536270	-4.264202
1	-7.597930	-2.807955	-3.305730
1	-7.554921	2.745507	3.473040
1	-7.313728	4.259125	1.532925
1	-7.416935	-4.022585	-1.538183
1	-7.173849	-4.389613	0.877753
1	-7.108710	4.492645	-0.597964
1	-6.876213	3.620471	-2.880714
1	-6.973518	-3.474622	2.826771
1	-6.724253	-1.567868	4.351587
1	-6.735616	1.763920	-3.925324
1	-6.546701	0.560795	4.325153
1	6.546701	-0.560568	4.325175
1	6.735619	-1.764123	-3.925230
1	6.724253	1.568100	4.351512
1	6.973517	3.474771	2.826599
1	6.876213	-3.620628	-2.880530

1	7.108703	-4.492691	-0.597739
1	7.173849	4.389657	0.877531
1	7.416933	4.022505	-1.538387
1	7.313728	-4.259044	1.533141
1	7.554922	-2.745321	3.473175
1	7.597930	2.807785	-3.305873
1	7.792663	0.536050	-4.264229

Nanotube (7,5) u05v07
B3LYP/STO-3G Energy: -5058.716462

6	7.105049	-0.050487	-3.849944
6	6.970669	1.302118	-3.662904
6	6.494203	-2.038281	4.001277
6	6.409804	-3.126810	3.168261
6	6.581628	3.663327	-1.826457
6	6.380268	4.207709	-0.576996
6	6.249679	-4.301639	0.393275
6	6.183626	-4.155697	-0.977564
6	5.930079	3.806899	2.380062
6	5.741076	2.986054	3.476119
6	6.027869	-2.254438	-3.286189
6	5.935068	-0.930040	-3.769501
6	5.421371	0.185304	4.498306
6	5.316878	-1.205217	4.255457
6	5.659301	1.908220	-3.423026
6	5.478268	3.067364	-2.568739
6	5.142328	-3.508578	2.545714
6	5.069958	-4.103893	1.219804
6	5.055815	4.236523	0.025219
6	4.840225	4.082189	1.462257
6	4.931987	-3.832846	-1.638527
6	4.865404	-2.945878	-2.814600
6	4.445083	2.403858	3.762726
6	4.292647	1.046413	4.327179
6	4.631100	-0.313257	-3.908402
6	4.498680	1.123749	-3.764250
6	4.022112	-1.777575	3.951856
6	3.938435	-2.957336	3.111483
6	4.144465	3.433711	-2.157142
6	3.935532	4.048892	-0.856520
6	3.792642	-4.175846	0.553761
6	3.727003	-4.062222	-0.894312
6	3.507815	3.826430	1.942113
6	3.309479	3.000434	3.121413
6	3.567846	-2.446288	-3.223908
6	3.457764	-1.140709	-3.826026
6	2.975391	0.441689	4.310235
6	2.841631	-0.986701	4.176947
6	3.173907	1.691843	-3.628140
6	2.998139	2.880493	-2.849139
6	2.645139	-3.350705	2.589379
6	2.571804	-3.998447	1.315499
6	2.584080	4.152711	-0.335589
6	2.369634	4.078129	1.075660
6	2.430820	-3.849136	-1.524730
6	2.354329	-3.074254	-2.723268
6	1.964984	2.530523	3.433947
6	1.797062	1.265147	4.076531
6	2.144288	-0.538890	-4.014559
6	2.007907	0.886038	-3.959945
6	1.530666	-1.571559	3.924599
6	1.434629	-2.782994	3.164177
6	1.654127	3.299842	-2.478889
6	1.449393	3.978576	-1.230537
6	1.279982	-4.144241	0.661304
6	1.213085	-4.108395	-0.775500
6	1.018363	3.905973	1.587490

6	0.817077	3.157740	2.803339
6	1.057548	-2.625458	-3.205511
6	0.957502	-1.363004	-3.901533
6	0.473719	0.669099	4.152036
6	0.340814	-0.771091	4.122782
6	0.686046	1.477750	-3.875971
6	0.513813	2.723966	-3.158609
6	0.142450	-3.222816	2.676828
6	0.069145	-3.946801	1.423952
6	0.107043	4.139950	-0.717772
6	-0.107054	4.140084	0.717003
6	-0.069154	-3.947066	-1.423224
6	-0.142452	-3.223314	-2.676235
6	-0.513813	2.724555	3.158105
6	-0.686038	1.478472	3.875700
6	-0.340804	-0.771859	-4.122647
6	-0.473709	0.668326	-4.152169
6	-0.957493	-1.362277	3.901787
6	-1.057546	-2.624859	3.205997
6	-0.817079	3.157213	-2.803928
6	-1.018372	3.905669	-1.588216
6	-1.213095	-4.108241	0.776258
6	-1.279991	-4.144354	-0.660539
6	-1.449403	3.978797	1.229798
6	-1.654130	3.300299	2.478280
6	-1.434627	-2.783580	-3.163671
6	-1.530657	-1.572289	-3.924323
6	-2.007897	0.886775	3.959794
6	-2.144277	-0.538142	4.014672
6	-1.797053	1.264387	-4.076782
6	-1.964981	2.529878	-3.434426
6	-2.354329	-3.073738	2.723839
6	-2.430827	-3.848835	1.525441
6	-2.369644	4.077907	-1.076417
6	-2.584091	4.152751	0.334817
6	-2.571813	-3.998672	-1.314762
6	-2.645141	-3.351176	-2.588767
6	-2.998139	2.881016	2.848614
6	-3.173899	1.692517	3.627845
6	-2.841621	-0.987478	-4.176790
6	-2.975379	0.440886	-4.310344
6	-3.457755	-1.139996	3.826259
6	-3.567842	-2.445679	3.224373
6	-3.309479	2.999840	-3.121979
6	-3.507823	3.826042	-1.942825
6	-3.727013	-4.062025	0.895062
6	-3.792653	-4.175916	-0.552990
6	-3.935543	4.049021	0.855769
6	-4.144471	3.434093	2.156513
6	-3.938434	-2.957904	-3.110951
6	-4.022103	-1.778309	-3.951557
6	-4.498671	1.124448	3.764076
6	-4.631090	-0.312529	3.908498
6	-4.292636	1.045606	-4.327408
6	-4.445079	2.403149	-3.763192
6	-4.865404	-2.945339	2.815161
6	-4.931995	-3.832507	1.639238
6	-4.840236	4.081876	-1.463017
6	-5.055828	4.236473	-0.026005
6	-5.069967	-4.104081	-1.219047
6	-5.142331	-3.509029	-2.545078
6	-5.478271	3.067824	2.568189
6	-5.659296	1.908852	3.422713
6	-5.316867	-1.206010	-4.255277
6	-5.421357	0.184467	-4.498389
6	-5.935059	-0.929336	3.769725
6	-6.027864	-2.253819	3.286644
6	-5.741074	2.985385	-3.476689
6	-5.930086	3.806415	-2.380773
6	-6.183636	-4.155457	0.978331

6	-6.249690	-4.301651	-0.392482
6	-6.380279	4.207761	0.576216
6	-6.581634	3.663628	1.825789
6	-6.409804	-3.127380	-3.167705
6	-6.494195	-2.039020	-4.000940
6	-6.970661	1.302797	3.662726
6	-7.105038	-0.049768	3.850024
1	8.101589	-0.506254	-3.931373
1	7.866264	1.933717	-3.600117
1	7.468719	-1.702937	4.382468
1	7.323227	-3.666599	2.886758
1	7.604311	3.558821	-2.210605
1	7.245574	4.529304	0.016914
1	7.227372	-4.433815	0.873829
1	7.111070	-4.174956	-1.564420
1	6.945152	4.137582	2.125729
1	6.610646	2.681415	4.072731
1	7.024781	-2.652737	-3.058587
1	6.425491	0.618768	4.588669
1	-6.425470	0.617912	-4.588843
1	-7.024779	-2.652160	3.059122
1	-6.610642	2.680635	-4.073248
1	-6.945164	4.137129	-2.126496
1	-7.111082	-4.174592	1.565189
1	-7.227384	-4.433904	-0.873011
1	-7.245589	4.529227	-0.017758
1	-7.604314	3.559193	2.209958
1	-7.323231	-3.667106	-2.886094
1	-7.468709	-1.703746	-4.382197
1	-7.866257	1.934383	3.599829
1	-8.101576	-0.505519	3.931549

Nanotube (7,5) u05v08
B3LYP/STO-3G Energy: -5134.009727

6	7.017394	-4.000180	1.017885
6	6.869902	-4.157960	-0.336802
6	6.810123	4.114880	0.927927
6	6.703741	3.594199	2.193525
6	6.533426	-2.971461	-3.089450
6	6.384823	-1.895973	-3.937010
6	6.433987	1.225219	4.043693
6	6.302094	-0.131406	4.255477
6	6.083956	1.084244	-4.307756
6	5.959331	2.360798	-3.793786
6	6.005913	-2.839024	3.008591
6	5.867463	-3.636898	1.851952
6	5.728654	4.077389	-1.345788
6	5.633083	4.202244	0.059482
6	5.561974	-4.012551	-0.979866
6	5.404422	-3.477255	-2.318375
6	5.414158	3.151388	2.725719
6	5.290037	2.030353	3.642540
6	5.090572	-1.254651	-4.117164
6	4.947009	0.181565	-4.337427
6	5.014953	-0.791140	4.118015
6	4.878272	-2.148322	3.562316
6	4.686268	2.850532	-3.301297
6	4.579679	3.747335	-2.133145
6	4.547587	-3.861091	1.295250
6	4.398469	-4.080875	-0.129734
6	4.333591	4.118173	0.693920
6	4.228789	3.614556	2.050319
6	4.086235	-3.106470	-2.775437
6	3.931351	-2.001189	-3.706464
6	3.984187	1.469400	3.890417
6	3.849617	0.045947	4.155781
6	3.642679	0.777425	-4.213042

6	3.512728	2.136641	-3.715070
6	3.554601	-2.607003	3.190284
6	3.393498	-3.513256	2.079822
6	3.272437	3.949440	-1.541178
6	3.153544	4.190431	-0.125145
6	3.072833	-4.026054	-0.709180
6	2.916326	-3.571619	-2.058690
6	2.919569	3.274933	2.568628
6	2.797716	2.217576	3.525389
6	2.605682	-1.458015	-3.940758
6	2.460988	-0.066145	-4.233597
6	2.523175	-0.553305	4.118881
6	2.377588	-1.904524	3.676904
6	2.192202	2.624368	-3.337605
6	2.072794	3.572148	-2.275514
6	2.062924	-3.779182	1.550475
6	1.905673	-4.078486	0.158577
6	1.841040	4.157810	0.507895
6	1.727842	3.739941	1.873401
6	1.586077	-3.253401	-2.555961
6	1.431578	-2.217918	-3.537304
6	1.479121	1.686961	3.840000
6	1.345261	0.297103	4.180128
6	1.138698	0.539902	-4.197323
6	1.006208	1.912686	-3.783436
6	1.051811	-2.420575	3.372156
6	0.896779	-3.402403	2.326186
6	0.762368	3.859742	-1.714576
6	0.649049	4.202123	-0.314614
6	0.579390	-4.076276	-0.430458
6	0.422256	-3.698118	-1.817880
6	0.420596	3.445760	2.427831
6	0.300678	2.430458	3.454090
6	0.112688	-1.697795	-3.827099
6	-0.031644	-0.305314	-4.200654
6	0.031641	-0.307040	4.200530
6	-0.112690	-1.699369	3.826408
6	-0.300678	2.431879	-3.453096
6	-0.420593	3.446761	-2.426421
6	-0.422257	-3.698868	1.816369
6	-0.579390	-4.076454	0.428791
6	-0.649045	4.201995	0.316335
6	-0.762365	3.859037	1.716157
6	-0.896780	-3.401444	-2.327574
6	-1.051812	-2.419187	-3.373141
6	-1.006208	1.911131	3.784215
6	-1.138701	0.538178	4.197541
6	-1.345263	0.298821	-4.180002
6	-1.479122	1.688541	-3.839307
6	-1.431580	-2.219373	3.536398
6	-1.586078	-3.254455	2.554632
6	-1.727839	3.740716	-1.871870
6	-1.841036	4.158023	-0.506192
6	-1.905673	-4.078422	-0.160244
6	-2.062924	-3.778544	-1.552019
6	-2.072791	3.571213	2.276975
6	-2.192202	2.622997	3.338676
6	-2.377589	-1.903011	-3.677677
6	-2.523177	-0.551612	-4.119101
6	-2.460991	-0.067884	4.233566
6	-2.605684	-1.459634	3.940160
6	-2.797716	2.219028	-3.524478
6	-2.919567	3.275995	-2.567287
6	-2.916328	-3.572469	2.057230
6	-3.072834	-4.026349	0.707534
6	-3.153540	4.190388	0.126861
6	-3.272433	3.948812	1.542794
6	-3.393498	-3.512402	-2.081257
6	-3.554601	-2.605691	-3.191346
6	-3.512728	2.135116	3.715938

6	-3.642682	0.775695	4.213353
6	-3.849620	0.047655	-4.155754
6	-3.984188	1.471001	-3.889810
6	-3.931354	-2.002712	3.705643
6	-4.086238	-3.107614	2.774166
6	-4.228786	3.615409	-2.048839
6	-4.333586	4.118471	-0.692234
6	-4.398469	-4.080934	0.128064
6	-4.547586	-3.860564	-1.296830
6	-4.579676	3.746465	2.134677
6	-4.686268	2.849178	3.302458
6	-4.878273	-2.146862	-3.563194
6	-5.014956	-0.789449	-4.118332
6	-4.947012	0.179786	4.337493
6	-5.090576	-1.256341	4.116647
6	-5.290038	2.031854	-3.641704
6	-5.414156	3.152519	-2.724428
6	-5.404425	-3.478213	2.316952
6	-5.561975	-4.012962	0.978223
6	-5.633078	4.202286	-0.057761
6	-5.728649	4.076850	1.347457
6	-5.867461	-3.636149	-1.853445
6	-6.005912	-2.837804	-3.009760
6	-5.959333	2.359242	3.794742
6	-6.083959	1.082477	4.308188
6	-6.302098	-0.129657	-4.255528
6	-6.433989	1.226884	-4.043187
6	-6.384826	-1.897591	3.936233
6	-6.533428	-2.972735	3.088235
6	-6.703738	3.595120	-2.192055
6	-6.810118	4.115284	-0.926243
6	-6.869902	-4.158113	0.335096
6	-7.017392	-3.999781	-1.019529
1	8.016024	-4.015001	1.476121
1	7.756699	-4.306091	-0.966578
1	7.795685	4.351682	0.503707
1	7.610713	3.418507	2.786400
1	7.537519	-3.368101	-2.892298
1	7.272654	-1.450042	-4.403736
1	7.434542	1.676067	4.046073
1	7.200931	-0.738717	4.423547
1	7.080632	0.703641	-4.565277
1	6.860363	2.971934	-3.653840
1	7.019080	-2.569140	3.332925
1	6.729312	4.006758	-1.791063
1	-6.729308	4.006040	1.792702
1	-7.019078	-2.567802	-3.333994
1	-6.860363	2.970435	3.655044
1	-7.080635	0.701770	4.565550
1	-7.200936	-0.736897	-4.423848
1	-7.434540	1.677734	-4.045389
1	-7.272657	-1.451851	4.403141
1	-7.537521	-3.369296	2.890923
1	-7.610710	3.419677	-2.785003
1	-7.795676	4.351920	-0.501928
1	-7.756699	-4.306507	0.964809
1	-8.016016	-4.014427	-1.477772

Nanotube (7,5) u05v09
B3LYP/STO-3G Energy: -5209.302727

C	7.132951	3.856287	-0.829331
C	6.730467	-4.452587	0.069322
C	6.609422	-4.267913	-1.285153
C	6.821974	3.428854	2.140524
C	6.655929	2.613779	3.237409
C	6.381736	-2.441964	-3.677067
C	6.296909	-1.180986	-4.228765

C	6.257757	-0.157433	4.365623
C	6.073817	-1.515870	4.199002
C	6.137156	1.766090	-3.712791
C	6.057662	2.836986	-2.797256
C	5.714236	-3.789110	2.275396
C	5.575237	-4.262355	0.951207
C	5.836617	3.933725	-0.150885
C	5.692602	3.765146	1.280682
C	5.323739	-3.917521	-1.891385
C	5.218348	-3.065382	-3.062729
C	5.343585	2.092582	3.594937
C	5.154339	0.769996	4.179610
C	5.039930	-0.451667	-4.245702
C	4.969723	1.006001	-4.055848
C	4.770142	-2.062227	3.869796
C	4.599374	-3.220480	2.972759
C	4.760956	3.252406	-2.297457
C	4.655081	3.832817	-0.974111
C	4.262348	-4.285503	0.337790
C	4.139679	-4.139399	-1.099608
C	4.373058	3.578648	1.837162
C	4.201540	2.756650	3.023519
C	3.928578	-2.529890	-3.426499
C	3.842090	-1.219068	-4.049514
C	3.826292	0.217158	4.236045
C	3.634342	-1.218163	4.108538
C	3.674407	1.602419	-3.796716
C	3.575546	2.767661	-2.952039
C	3.269931	-3.512420	2.475270
C	3.103136	-4.097857	1.168306
C	3.343489	3.982904	-0.380706
C	3.203768	3.892892	1.042527
C	2.830977	-3.885208	-1.665578
C	2.724270	-3.104704	-2.861109
C	2.864175	2.347101	3.409624
C	2.677135	1.085467	4.055692
C	2.541652	-0.573411	-4.150626
C	2.459742	0.851312	-4.071011
C	2.288432	-1.731105	3.892702
C	2.105972	-2.912256	3.110823
C	2.269995	3.215780	-2.488847
C	2.158017	3.862292	-1.216374
C	1.776370	-4.167718	0.570147
C	1.641951	-4.102351	-0.854320
C	1.875197	3.765529	1.623585
C	1.707663	3.024150	2.839332
C	1.419742	-2.614588	-3.280820
C	1.330305	-1.357832	-3.970513
C	1.332839	0.545774	4.198397
C	1.140294	-0.878902	4.159125
C	1.162983	1.485700	-3.890894
C	1.071154	2.705324	-3.128321
C	0.770599	-3.278426	2.664678
C	0.606079	-3.953091	1.399147
C	0.846606	4.064025	-0.626700
C	0.709614	4.055516	0.812671
C	0.331852	-3.897665	-1.442828
C	0.223222	-3.177761	-2.693422
C	0.377872	2.651221	3.273610
C	0.193036	1.411285	3.999893
C	0.040350	-0.722165	-4.130802
C	-0.040358	0.723156	-4.130639
C	-0.193047	-1.412248	3.999560
C	-0.377881	-2.652017	3.272984
C	-0.223221	3.178410	-2.692676
C	-0.331848	3.898016	-1.441907
C	-0.709611	-4.055729	0.811713
C	-0.846601	-4.063892	-0.627668
C	-0.606078	3.952753	1.400082
C	-0.770602	3.277782	2.665455

C	-1.071153	-2.704579	-3.128955
C	-1.162985	-1.484765	-3.891238
C	-1.140304	0.877904	4.159327
C	-1.332847	-0.546788	4.198264
C	-1.330308	1.358784	-3.970197
C	-1.419740	2.615389	-3.280209
C	-1.707665	-3.024846	2.838615
C	-1.875195	-3.765944	1.622690
C	-1.641939	4.102575	-0.853351
C	-1.776358	4.167596	0.571137
C	-2.158011	-3.862023	-1.217292
C	-2.269988	-3.215191	-2.489606
C	-2.105976	2.911504	3.111503
C	-2.288435	1.730166	3.893092
C	-2.459743	-0.850333	-4.071185
C	-2.541655	0.574404	-4.150464
C	-2.677141	-1.086443	4.055411
C	-2.864180	-2.347923	3.409053
C	-2.724262	3.105405	-2.860367
C	-2.830967	3.885631	-1.664661
C	-3.203766	-3.893173	1.041599
C	-3.343485	-3.982843	-0.381653
C	-3.103128	4.097593	1.169277
C	-3.269932	3.511826	2.476082
C	-3.575545	-2.766959	-2.952686
C	-3.674411	-1.601508	-3.797064
C	-3.634354	1.217173	4.108788
C	-3.826302	-0.218171	4.235957
C	-3.842097	1.220037	-4.049180
C	-3.928583	2.530718	-3.425881
C	-4.201548	-2.757388	3.022852
C	-4.373064	-3.579122	1.836310
C	-4.139671	4.139718	-1.098629
C	-4.262338	4.285480	0.338802
C	-4.655079	-3.832627	-0.975026
C	-4.760953	-3.251882	-2.298233
C	-4.599386	3.219778	2.973496
C	-4.770150	2.061295	3.870252
C	-4.969730	-1.005039	-4.056052
C	-5.039941	0.452688	-4.245541
C	-5.154347	-0.770995	4.179397
C	-5.343594	-2.093460	3.594419
C	-5.218344	3.066139	-3.061983
C	-5.323724	3.918045	-1.890457
C	-5.692603	-3.765503	1.279788
C	-5.836613	-3.933744	-0.151830
C	-5.575219	4.262189	0.952207
C	-5.714227	3.788596	2.276281
C	-6.057656	-2.836347	-2.797928
C	-6.137150	-1.765213	-3.713193
C	-6.073823	1.514865	4.199291
C	-6.257764	0.156382	4.365594
C	-6.296913	1.181977	-4.228384
C	-6.381740	2.442843	-3.676403
C	-6.655936	-2.614572	3.236768
C	-6.821979	-3.429405	2.139700
C	-6.609410	4.268350	-1.284144
C	-6.730452	4.452670	0.070357
C	-7.132944	-3.856138	-0.830258
C	-7.240866	-3.352166	-2.101236
H	8.227581	3.209050	-2.562261
H	8.039818	4.123593	-0.271551
H	7.717272	-4.618164	0.523508
H	7.505542	-4.291206	-1.918731
H	7.834131	3.722756	1.834473
H	7.537903	2.268154	3.792059
H	7.363433	-2.923029	-3.580103
H	7.213449	-0.677618	-4.562854
H	7.273567	0.235185	4.502186
H	6.947652	-2.180189	4.207528

H	7.130717	1.378733	-3.972081
H	6.728407	-3.651494	2.671573
H	-6.728408	3.650894	2.672408
H	-7.130715	-1.377798	-3.972381
H	-6.947672	2.179167	4.207912
H	-7.273587	-0.236262	4.501998
H	-7.213475	0.678658	-4.562483
H	-7.363450	2.923838	-3.579255
H	-7.537913	-2.269076	3.791493
H	-7.834137	-3.723239	1.833580
H	-7.505497	4.291908	-1.917767
H	-7.717227	4.618243	0.524604
H	-8.039810	-4.123584	-0.272546
H	-8.227571	-3.208463	-2.563033

Nanotube (7,5) u05v10
B3LYP/STO-3G Energy: -5284.595426

C	-7.144222	-3.730230	-1.656649
C	-6.963503	4.075436	1.337548
C	-6.878100	4.248131	-0.020907
C	-6.747618	-4.069109	1.315028
C	-6.570168	-3.557049	2.580188
C	-6.668589	3.108735	-2.807487
C	-6.563665	2.036298	-3.666803
C	-6.222101	-1.155373	4.374616
C	-6.086699	0.206019	4.559965
C	-6.303067	-0.936902	-3.928537
C	-6.163576	-2.202194	-3.321816
C	-5.860006	2.908495	3.276863
C	-5.776399	3.708894	2.116275
C	-5.824358	-3.931381	-1.052149
C	-5.637795	-4.129191	0.369715
C	-5.601147	4.111854	-0.724750
C	-5.505438	3.593883	-2.076580
C	-5.263382	-3.093370	3.027270
C	-5.096522	-1.960138	3.928355
C	-5.286310	1.380448	-3.897355
C	-5.168234	-0.071930	-4.091636
C	-4.811878	0.868974	4.352858
C	-4.706044	2.223460	3.781544
C	-4.839377	-2.685889	-2.977818
C	-4.673581	-3.581006	-1.851556
C	-4.483817	3.938313	1.500998
C	-4.400133	4.168370	0.072358
C	-4.306108	-4.041078	0.923390
C	-4.120415	-3.543676	2.275908
C	-4.211473	3.217080	-2.594024
C	-4.105442	2.114766	-3.536263
C	-3.784988	-1.389458	4.094935
C	-3.642498	0.036026	4.340433
C	-3.849011	-0.668238	-4.027086
C	-3.690079	-2.008168	-3.515392
C	-3.402622	2.685175	3.348481
C	-3.294487	3.590761	2.231474
C	-3.339586	-3.831035	-1.349249
C	-3.155024	-4.099474	0.046629
C	-3.102600	4.115783	-0.567877
C	-3.008582	3.670291	-1.925583
C	-2.784450	-3.194691	2.721242
C	-2.615689	-2.135731	3.667689
C	-2.791203	1.563947	-3.828620
C	-2.665855	0.171315	-4.123849
C	-2.321448	0.638979	4.236480
C	-2.201305	1.988253	3.783684
C	-2.358898	-2.513767	-3.215927
C	-2.186883	-3.459764	-2.155652
C	-1.990004	3.860750	1.642546
C	-1.896538	4.162751	0.246484

C	-1.812561	-4.072019	0.607711
C	-1.627364	-3.655978	1.966945
C	-1.702940	3.349720	-2.483971
C	-1.597233	2.317690	-3.475439
C	-1.285486	-1.598938	3.913290
C	-1.138749	-0.208150	4.245160
C	-1.345908	-0.441458	-4.144086
C	-1.195358	-1.812057	-3.729832
C	-0.892753	2.508493	3.418873
C	-0.788107	3.487837	2.365755
C	-0.851089	-3.758626	-1.669667
C	-0.666180	-4.105447	-0.280177
C	-0.598356	4.162045	-0.402828
C	-0.505548	3.787289	-1.796780
C	-0.295432	-3.351898	2.447932
C	-0.125251	-2.336967	3.465823
C	-0.294297	1.791735	-3.823245
C	-0.171980	0.400279	-4.203574
C	0.171983	0.400629	4.203540
C	0.294298	1.792053	3.823096
C	0.125253	-2.337256	-3.465632
C	0.295432	-3.352104	-2.447657
C	0.505545	3.787440	1.796466
C	0.598353	4.162080	0.402484
C	0.666177	-4.105425	0.280515
C	0.851088	-3.758486	1.669976
C	0.788106	3.487641	-2.366044
C	0.892754	2.508209	-3.419080
C	1.195360	-1.811745	3.729979
C	1.345911	-0.441112	4.144119
C	1.138752	-0.208503	-4.245140
C	1.285488	-1.599265	-3.913157
C	1.597234	2.317981	3.475245
C	1.702939	3.349930	2.483694
C	1.627363	-3.656145	-1.966644
C	1.812558	-4.072073	-0.607376
C	1.896534	4.162735	-0.246829
C	1.990002	3.860617	-1.642865
C	2.186882	-3.459585	2.155935
C	2.358899	-2.513498	3.216130
C	2.201308	1.987939	-3.783845
C	2.321452	0.638626	-4.236527
C	2.665858	0.171660	4.123829
C	2.791205	1.564268	3.828487
C	2.615690	-2.136038	-3.667511
C	2.784450	-3.194922	-2.720978
C	3.008579	3.670458	1.925279
C	3.102596	4.115839	0.567537
C	3.155022	-4.099483	-0.046291
C	3.339584	-3.830926	1.349564
C	3.294486	3.590580	-2.231769
C	3.402625	2.684898	-3.348698
C	3.690080	-2.007874	3.515551
C	3.849013	-0.667901	4.027132
C	3.642502	0.035664	-4.340427
C	3.784990	-1.389800	-4.094815
C	4.105443	2.115065	3.536084
C	4.211472	3.217303	2.593757
C	4.120414	-3.543873	-2.275616
C	4.306106	-4.041164	-0.923057
C	4.400129	4.168377	-0.072701
C	4.483815	3.938198	-1.501322
C	4.673580	-3.580856	1.851849
C	4.839378	-2.685642	2.978033
C	4.706048	2.223143	-3.781715
C	4.811882	0.868609	-4.352918
C	5.168237	-0.071587	4.091630
C	5.286311	1.380776	3.897232
C	5.096524	-1.960469	-3.928189
C	5.263382	-3.093631	-3.027014

C	5.505436	3.594068	2.076284
C	5.601143	4.111932	0.724412
C	5.637792	-4.129233	-0.369376
C	5.824357	-3.931302	1.052472
C	5.776398	3.708722	-2.116574
C	5.860012	2.908212	-3.277083
C	6.163576	-2.201918	3.321988
C	6.303069	-0.936573	3.928600
C	6.086702	0.205637	-4.559969
C	6.222102	-1.155741	-4.374513
C	6.563666	2.036611	3.666628
C	6.668586	3.108981	2.807229
C	6.570166	-3.557279	-2.579897
C	6.747616	-4.069235	-1.314694
C	6.878097	4.248155	0.020561
C	6.963501	4.075337	-1.337878
C	7.144220	-3.730103	1.656955
C	7.308234	-2.922135	2.752711
H	-8.313213	-2.701653	-3.138265
H	-8.024124	-4.164618	-1.164625
H	-7.940517	4.083238	1.840460
H	-7.793214	4.400243	-0.607801
H	-7.759655	-4.314868	0.968766
H	-7.443053	-3.400886	3.227225
H	-7.660102	3.515246	-2.570378
H	-7.474189	1.604341	-4.102037
H	-7.219831	-1.609440	4.429760
H	-6.980058	0.811506	4.760783
H	-7.314906	-0.531615	-4.056692
H	-6.856577	2.635564	3.646821
H	6.856586	2.635221	-3.646992
H	7.314908	-0.531276	4.056721
H	6.980061	0.811107	-4.760835
H	7.219831	-1.609812	-4.429623
H	7.474190	1.604690	4.101897
H	7.660100	3.515475	2.570089
H	7.443052	-3.401171	-3.226947
H	7.759652	-4.314965	-0.968411
H	7.793209	4.400319	0.607442
H	7.940514	4.083093	-1.840791
H	8.024121	-4.164536	1.164971
H	8.313212	-2.701400	3.138484

Nanotube (7,5) u05v11
B3LYP/STO-3G Energy: -5359.897538

6	2.065684	7.301269	-3.619732
6	1.085873	7.760162	-2.761457
6	6.812827	4.110699	2.187571
6	7.185110	3.730266	0.911260
6	0.000888	8.082341	0.031135
6	0.075290	7.876258	1.402921
6	6.692161	3.683720	-2.062754
6	5.920902	4.005577	-3.176588
6	1.499952	6.651745	3.763567
6	2.517912	5.868064	4.308372
6	3.398992	5.249213	-4.217614
6	2.145642	5.889406	-3.957280
6	4.881271	4.085908	3.805987
6	5.746191	3.412292	2.881809
6	0.090833	6.860808	-2.204910
6	-0.462212	7.039854	-0.851669
6	6.552055	2.608625	0.245559
6	6.338010	2.577205	-1.214370
6	-0.334968	6.627383	1.991445
6	0.338929	6.046460	3.174987
6	4.766427	3.228817	-3.531982
6	3.534825	3.845516	-4.103516
6	2.425614	4.437799	4.327735

6	3.613874	3.554829	4.133978
6	0.983944	5.078159	-3.698389
6	-0.066544	5.580647	-2.833501
6	5.362931	2.118502	2.379247
6	5.790420	1.703675	1.057695
6	-1.191926	5.954664	-0.252432
6	-1.147144	5.760837	1.183618
6	5.427099	1.605151	-1.759796
6	4.652677	1.923558	-2.942107
6	0.083971	4.670174	3.505941
6	1.123383	3.866147	4.113432
6	2.324450	3.037404	-4.138457
6	1.038968	3.665317	-3.995166
6	3.373634	2.142765	3.864635
6	4.286168	1.407019	3.031053
6	-1.088988	4.656024	-2.368574
6	-1.688765	4.865173	-1.082329
6	5.179915	0.522302	0.465678
6	5.030966	0.451986	-0.961742
6	-1.672446	4.523220	1.746919
6	-1.078669	3.991991	2.945839
6	3.563174	1.033921	-3.334056
6	2.402469	1.594817	-3.987595
6	0.926694	2.424649	4.227679
6	2.080051	1.551895	4.151507
6	-0.149419	2.850534	-3.810590
6	-1.248337	3.374309	-3.018733
6	3.942776	0.070046	2.584793
6	4.433505	-0.392069	1.295610
6	-2.499759	3.823402	-0.497100
6	-2.520953	3.673897	0.951809
6	4.198686	-0.572185	-1.540608
6	3.477622	-0.284942	-2.774962
6	-1.395472	2.652895	3.364027
6	-0.380811	1.865182	4.055259
6	1.211150	0.797428	-4.122027
6	-0.090833	1.442683	-4.074992
6	1.885048	0.137761	3.971467
6	2.855551	-0.626159	3.207270
6	-2.290521	2.482698	-2.580283
6	-2.950472	2.729835	-1.315710
6	3.864547	-1.577805	0.708067
6	3.776512	-1.685916	-0.730511
6	-3.061139	2.468418	1.528865
6	-2.518476	1.970212	2.770696
6	2.410015	-1.169202	-3.187810
6	1.282201	-0.631066	-3.905449
6	-0.573476	0.436191	4.196553
6	0.573476	-0.436191	4.196553
6	-1.282201	0.631066	-3.905449
6	-2.410015	1.169202	-3.187810
6	2.518476	-1.970212	2.770696
6	3.061139	-2.468418	1.528865
6	-3.776512	1.685916	-0.730511
6	-3.864547	1.577805	0.708067
6	2.950472	-2.729835	-1.315710
6	2.290521	-2.482698	-2.580283
6	-2.855551	0.626159	3.207270
6	-1.885048	-0.137761	3.971467
6	0.090833	-1.442683	-4.074992
6	-1.211150	-0.797428	-4.122027
6	0.380811	-1.865182	4.055259
6	1.395472	-2.652895	3.364027
6	-3.477622	0.284942	-2.774962
6	-4.198686	0.572185	-1.540608
6	2.520953	-3.673897	0.951809
6	2.499759	-3.823402	-0.497100
6	-4.433505	0.392069	1.295610
6	-3.942776	-0.070046	2.584793
6	1.248337	-3.374309	-3.018733

6	0.149419	-2.850534	-3.810590
6	-2.080051	-1.551895	4.151507
6	-0.926694	-2.424649	4.227679
6	-2.402469	-1.594817	-3.987595
6	-3.563174	-1.033921	-3.334056
6	1.078669	-3.991991	2.945839
6	1.672446	-4.523220	1.746919
6	-5.030966	-0.451986	-0.961742
6	-5.179915	-0.522302	0.465678
6	1.688765	-4.865173	-1.082329
6	1.088988	-4.656024	-2.368574
6	-4.286168	-1.407019	3.031053
6	-3.373634	-2.142765	3.864635
6	-1.038968	-3.665317	-3.995166
6	-2.324450	-3.037404	-4.138457
6	-1.123383	-3.866147	4.113432
6	-0.083971	-4.670174	3.505941
6	-4.652677	-1.923558	-2.942107
6	-5.427099	-1.605151	-1.759796
6	1.147144	-5.760837	1.183618
6	1.191926	-5.954664	-0.252432
6	-5.790420	-1.703675	1.057695
6	-5.362931	-2.118502	2.379247
6	0.066544	-5.580647	-2.833501
6	-0.983944	-5.078159	-3.698389
6	-3.613874	-3.554829	4.133978
6	-2.425614	-4.437799	4.327735
6	-3.534825	-3.845516	-4.103516
6	-4.766427	-3.228817	-3.531982
6	-0.338929	-6.046460	3.174987
6	0.334968	-6.627383	1.991445
6	-6.338010	-2.577205	-1.214370
6	-6.552055	-2.608625	0.245559
6	0.462212	-7.039854	-0.851669
6	-0.090833	-6.860808	-2.204910
6	-5.746191	-3.412292	2.881809
6	-4.881271	-4.085908	3.805987
6	-2.145642	-5.889406	-3.957280
6	-3.398992	-5.249213	-4.217614
6	-2.517912	-5.868064	4.308372
6	-1.499952	-6.651745	3.763567
6	-5.920902	-4.005577	-3.176588
6	-6.692161	-3.683720	-2.062754
6	-0.075290	-7.876258	1.402921
6	-0.000888	-8.082341	0.031135
6	-7.185110	-3.730266	0.911260
6	-6.812827	-4.110699	2.187571
6	-1.085873	-7.760162	-2.761457
6	-2.065684	-7.301269	-3.619732
1	2.876093	7.969788	-3.940924
1	1.123904	8.798823	-2.408866
1	7.220810	5.029763	2.629790
1	7.892779	4.354723	0.350963
1	0.437775	8.994966	-0.393359
1	0.570629	8.630734	2.027602
1	7.482990	4.376334	-1.748462
1	6.124909	4.944875	-3.706710
1	1.670383	7.729078	3.643250
1	3.458644	6.353935	4.597934
1	4.293622	5.883863	-4.253389
1	5.115526	5.130512	4.046994
1	-5.115526	-5.130512	4.046994
1	-4.293622	-5.883863	-4.253389
1	-3.458644	-6.353935	4.597934
1	-1.670383	-7.729078	3.643250
1	-6.124909	-4.944875	-3.706710
1	-7.482990	-4.376334	-1.748462
1	-0.570629	-8.630734	2.027602
1	-0.437775	-8.994966	-0.393359
1	-7.892779	-4.354723	0.350963

1	-7.220810	-5.029763	2.629790
1	-1.123904	-8.798823	-2.408866
1	-2.876093	-7.969788	-3.940924

Nanotube (7,5) u06v00
B3LYP/STO-3G Energy: -5435.197388

6	-7.551063	-1.060819	-3.784098
6	-7.405196	-2.318857	-3.234696
6	-7.073712	2.956428	3.257015
6	-6.987877	3.786167	2.155638
6	-7.014665	-4.095584	-0.832354
6	-6.824225	-4.285759	0.529684
6	-6.796841	4.183547	-0.826860
6	-6.711306	3.674114	-2.118632
6	-6.423209	-3.105702	3.276301
6	-6.261080	-2.009246	4.121956
6	-6.506794	1.230520	-3.841754
6	-6.396914	-0.191530	-3.949806
6	-5.988402	0.970438	4.364836
6	-5.896999	2.259360	3.747901
6	-6.100289	-2.823888	-2.844267
6	-5.916655	-3.718772	-1.690085
6	-5.723391	4.013570	1.480529
6	-5.637219	4.233339	0.025578
6	-5.520422	-4.141318	1.126595
6	-5.326617	-3.597806	2.488985
6	-5.461064	3.208312	-2.653854
6	-5.371644	2.027334	-3.558702
6	-4.990621	-1.356815	4.258426
6	-4.862048	0.118507	4.440062
6	-5.092739	-0.801269	-3.893966
6	-4.947640	-2.142284	-3.359838
6	-4.610846	2.737646	3.309272
6	-4.526453	3.642395	2.178987
6	-4.588825	-3.924550	-1.177163
6	-4.391067	-4.160723	0.239805
6	-4.353734	4.121855	-0.616644
6	-4.266480	3.626977	-1.976046
6	-4.006409	-3.188947	2.885499
6	-3.835594	-2.078928	3.799369
6	-4.056480	1.450697	-3.795216
6	-3.923891	0.037364	-4.024370
6	-3.543544	0.712229	4.267911
6	-3.420919	2.050573	3.756326
6	-3.611309	-2.633702	-3.061908
6	-3.431915	-3.565388	-1.986457
6	-3.222317	3.897111	1.585379
6	-3.135682	4.176949	0.180184
6	-3.039544	-4.106710	0.783461
6	-2.846155	-3.653505	2.134252
6	-2.955370	3.281488	-2.519086
6	-2.857505	2.209096	-3.481748
6	-2.498115	-1.531137	4.004270
6	-2.355110	-0.122186	4.294526
6	-2.605484	-0.573343	-4.044869
6	-2.456433	-1.946270	-3.597172
6	-2.115901	2.567491	3.382771
6	-2.022744	3.537447	2.305561
6	-2.099096	-3.856005	-1.510857
6	-1.904126	-4.170774	-0.102049
6	-1.847571	4.163575	-0.470458
6	-1.763653	3.739046	-1.862735
6	-1.520024	-3.336229	2.595863
6	-1.346862	-2.275752	3.582154
6	-1.563760	1.668412	-3.811180
6	-1.441034	0.257788	-4.141737
6	-1.052572	0.486776	4.221195

6	-0.932995	1.872031	3.798082
6	-1.139272	-2.464662	-3.334012
6	-0.962398	-3.460639	-2.297939
6	-0.735799	3.829864	1.727702
6	-0.650107	4.179741	0.326527
6	-0.573213	-4.150915	0.447817
6	-0.379271	-3.762321	1.825141
6	-0.470118	3.415060	-2.422047
6	-0.371902	2.396652	-3.437217
6	-0.023511	-1.739055	3.813366
6	0.125092	-0.353100	4.178516
6	-0.125091	-0.353093	-4.178516
6	0.023512	-1.739048	-3.813368
6	0.371902	2.396647	3.437221
6	0.470118	3.415056	2.422052
6	0.379270	-3.762318	-1.825146
6	0.573212	-4.150915	-0.447823
6	0.650106	4.179743	-0.326520
6	0.735798	3.829868	-1.727696
6	0.962397	-3.460643	2.297934
6	1.139272	-2.464668	3.334008
6	0.932995	1.872037	-3.798079
6	1.052573	0.486783	-4.221193
6	1.441035	0.257781	4.141737
6	1.563761	1.668406	3.811182
6	1.346862	-2.275746	-3.582156
6	1.520024	-3.336225	-2.595867
6	1.763651	3.739044	1.862742
6	1.847570	4.163576	0.470465
6	1.904125	-4.170776	0.102043
6	2.099096	-3.856009	1.510851
6	2.022743	3.537452	-2.305555
6	2.115901	2.567497	-3.382766
6	2.456433	-1.946277	3.597168
6	2.605485	-0.573349	4.044867
6	2.355111	-0.122179	-4.294524
6	2.498116	-1.531131	-4.004270
6	2.857505	2.209091	3.481750
6	2.955370	3.281485	2.519091
6	2.846155	-3.653503	-2.134257
6	3.039543	-4.106711	-0.783467
6	3.135680	4.176952	-0.180177
6	3.222316	3.897116	-1.585373
6	3.431914	-3.565393	1.986451
6	3.611309	-2.633707	3.061903
6	3.420919	2.050580	-3.756321
6	3.543546	0.712236	-4.267906
6	3.923893	0.037357	4.024367
6	4.056481	1.450692	3.795215
6	3.835594	-2.078922	-3.799369
6	4.006409	-3.188944	-2.885502
6	4.266479	3.626976	1.976052
6	4.353733	4.121858	0.616651
6	4.391066	-4.160727	-0.239812
6	4.588824	-3.924555	1.177157
6	4.526452	3.642402	-2.178980
6	4.610846	2.737653	-3.309266
6	4.947641	-2.142290	3.359831
6	5.092740	-0.801275	3.893960
6	4.862050	0.118514	-4.440057
6	4.990622	-1.356809	-4.258424
6	5.371644	2.027330	3.558703
6	5.461063	3.208310	2.653858
6	5.326617	-3.597805	-2.488990
6	5.520421	-4.141322	-1.126601
6	5.637218	4.233344	-0.025572
6	5.723390	4.013577	-1.480523
6	5.916655	-3.718778	1.690078
6	6.100289	-2.823893	2.844259
6	5.896999	2.259367	-3.747895

6	5.988404	0.970445	-4.364829
6	6.396916	-0.191536	3.949800
6	6.506796	1.230514	3.841751
6	6.261080	-2.009241	-4.121956
6	6.423209	-3.105700	-3.276304
6	6.711306	3.674114	2.118637
6	6.796840	4.183551	0.826867
6	6.824224	-4.285767	-0.529691
6	7.014664	-4.095592	0.832347
6	6.987876	3.786177	-2.155632
6	7.073712	2.956437	-3.257009
6	7.405197	-2.318862	3.234685
6	7.551065	-1.060824	3.784088
1	-8.553772	-0.651324	-3.969246
1	-8.299981	-2.905452	-2.989628
1	-8.054595	2.706533	3.684601
1	-7.908208	4.193306	1.717400
1	-8.037285	-4.090148	-1.230585
1	-7.701027	-4.424351	1.175309
1	-7.786903	4.405692	-0.408675
1	-7.637409	3.505510	-2.683354
1	-7.435495	-3.490047	3.096868
1	-7.151728	-1.561453	4.581594
1	-7.513122	1.653935	-3.728921
1	-6.992611	0.565268	4.544330
1	6.992613	0.565276	-4.544324
1	7.513124	1.653931	3.728919
1	7.151729	-1.561448	-4.581593
1	7.435494	-3.490046	-3.096873
1	7.637410	3.505508	2.683358
1	7.786902	4.405698	0.408682
1	7.701025	-4.424360	-1.175317
1	8.037284	-4.090159	1.230578
1	7.908206	4.193317	-1.717395
1	8.054595	2.706544	-3.684596
1	8.299982	-2.905456	2.989615
1	8.553774	-0.651328	3.969235

Nanotube (7,5) u06v01
B3LYP/STO-3G Energy: -5510.496510

6	-7.503518	-0.012429	-4.156523
6	-7.376936	-1.369288	-3.942364
6	-7.301600	2.069433	3.689329
6	-7.177124	3.152830	2.841704
6	-7.077087	-3.704372	-2.060874
6	-6.938581	-4.237610	-0.787821
6	-6.876174	4.296953	0.068387
6	-6.740199	4.133280	-1.305723
6	-6.642168	-3.800725	2.182026
6	-6.512696	-2.957859	3.283611
6	-6.462367	2.208593	-3.585525
6	-6.344856	0.861969	-4.048084
6	-6.253377	-0.141916	4.289213
6	-6.141906	1.260659	4.026996
6	-6.086283	-1.968236	-3.643112
6	-5.946322	-3.129294	-2.752569
6	-5.888553	3.536647	2.293768
6	-5.748856	4.120893	0.948440
6	-5.657101	-4.262209	-0.125462
6	-5.515405	-4.085700	1.335223
6	-5.467994	3.811567	-1.895073
6	-5.339922	2.899457	-3.065898
6	-5.247743	-2.372096	3.628004
6	-5.128438	-0.993395	4.184310
6	-5.041997	0.247868	-4.100388
6	-4.915431	-1.186807	-3.923200
6	-4.841327	1.826178	3.773067

6	-4.717505	2.990660	2.917282
6	-4.638810	-3.473394	-2.261669
6	-4.495206	-4.066919	-0.945786
6	-4.442143	4.170659	0.347421
6	-4.301974	4.037732	-1.089199
6	-4.211516	-3.803794	1.871544
6	-4.076253	-2.963268	3.043304
6	-4.016075	2.391912	-3.390602
6	-3.871398	1.082195	-3.965847
6	-3.805963	-0.385277	4.216908
6	-3.667331	1.038511	4.070629
6	-3.591730	-1.749196	-3.710004
6	-3.452845	-2.927566	-2.906442
6	-3.393097	3.380536	2.457427
6	-3.255007	4.012139	1.176505
6	-3.165752	-4.165142	-0.356524
6	-3.023909	-4.071725	1.069610
6	-2.969948	3.832043	-1.652516
6	-2.831350	3.037329	-2.848211
6	-2.747523	-2.495002	3.427684
6	-2.617547	-1.207837	4.070898
6	-2.550725	0.485777	-4.088058
6	-2.416690	-0.954906	-4.003489
6	-2.350086	1.624339	3.889539
6	-2.219597	2.838757	3.104192
6	-2.137215	-3.343486	-2.471976
6	-1.996099	-4.011574	-1.187553
6	-1.942954	4.159599	0.592860
6	-1.804563	4.104313	-0.857450
6	-1.714440	-3.893969	1.645327
6	-1.580034	-3.118088	2.873010
6	-1.523089	2.588577	-3.253681
6	-1.384160	1.305639	-3.924839
6	-1.313802	-0.610094	4.202353
6	-1.181582	0.836611	4.153590
6	-1.109653	-1.535615	-3.834406
6	-0.971427	-2.769838	-3.087620
6	-0.913306	3.262549	2.669784
6	-0.776819	3.963128	1.411034
6	-0.687305	-4.148031	-0.602670
6	-0.546735	-4.122985	0.835575
6	-0.491323	3.926582	-1.431945
6	-0.350166	3.192608	-2.664202
6	-0.267408	-2.667351	3.279896
6	-0.134448	-1.419902	3.989067
6	-0.068212	0.713447	-4.061090
6	0.068211	-0.720333	-4.059886
6	0.134442	1.426667	3.986670
6	0.267405	2.672917	3.275394
6	0.350167	-3.197130	-2.658811
6	0.491327	-3.929010	-1.425309
6	0.546738	4.124397	0.828606
6	0.687309	4.147000	-0.609679
6	0.776821	-3.960721	1.417728
6	0.913306	-3.258007	2.675287
6	0.971428	2.764590	-3.092288
6	1.109652	1.529108	-3.836990
6	1.181576	-0.829565	4.154996
6	1.313795	0.617220	4.201326
6	1.384159	-1.312295	-3.922639
6	1.523088	-2.594098	-3.249315
6	1.580032	3.122963	2.867747
6	1.714441	3.896758	1.638747
6	1.804567	-4.105760	-0.850513
6	1.942958	-4.158579	0.599889
6	1.996103	4.009543	-1.194328
6	2.137218	3.339278	-2.477616
6	2.219596	-2.833478	3.108979
6	2.350081	-1.617737	3.892277
6	2.416689	0.948114	-4.005096

6	2.550723	-0.492709	-4.087240
6	2.617541	1.214740	4.068867
6	2.747519	2.500817	3.423480
6	2.831350	-3.042162	-2.843086
6	2.969950	-3.834842	-1.646042
6	3.023912	4.073530	1.062730
6	3.165756	4.164518	-0.363560
6	3.255011	-4.010120	1.183282
6	3.393097	-3.376346	2.463132
6	3.452847	2.922621	-2.911377
6	3.591730	1.742897	-3.712950
6	3.667326	-1.031605	4.072385
6	3.805957	0.392428	4.216266
6	3.871396	-1.088920	-3.964028
6	4.016075	-2.397665	-3.386573
6	4.076251	2.968430	3.038309
6	4.211518	3.806962	1.865122
6	4.301977	-4.039568	-1.082376
6	4.442147	-4.170045	0.354468
6	4.495210	4.065290	-0.952652
6	4.638813	3.469535	-2.267528
6	4.717505	-2.985691	2.922328
6	4.841324	-1.819770	3.776151
6	4.915430	1.180149	-3.925202
6	5.041996	-0.254822	-4.099976
6	5.128431	1.000490	4.182652
6	5.247738	2.378249	3.624015
6	5.339922	-2.904660	-3.061014
6	5.467996	-3.814775	-1.888636
6	5.515408	4.087950	1.328323
6	5.657106	4.261968	-0.132660
6	5.748860	-4.119254	0.955400
6	5.888554	-3.532727	2.299737
6	5.946326	3.124603	-2.757845
6	6.086284	1.962047	-3.646431
6	6.141902	-1.253824	4.029134
6	6.253371	0.149189	4.288994
6	6.344853	-0.868835	-4.046646
6	6.462365	-2.214678	-3.581817
6	6.512693	2.963424	3.278631
6	6.642169	3.804414	2.175614
6	6.740203	-4.135476	-1.298738
6	6.876179	-4.296804	0.075649
6	6.938586	4.236237	-0.794973
6	7.077092	3.700844	-2.067121
6	7.177124	-3.147983	2.847023
6	7.301598	-2.063162	3.692826
6	7.376936	1.362596	-3.944681
6	7.503515	0.005379	-4.156561
1	-8.498616	0.439168	-4.271739
1	-8.278879	-1.992874	-3.892857
1	-8.296887	1.725652	4.003415
1	-8.081321	3.666164	2.489931
1	-8.083353	-3.589513	-2.483497
1	-7.838563	-4.530870	-0.232072
1	-7.881845	4.411883	0.492491
1	-7.643364	4.120896	-1.929520
1	-7.646274	-4.119613	1.874287
1	-7.419718	-2.635430	3.811217
1	-7.473073	2.598033	-3.408059
1	-7.262607	-0.572129	4.323494
1	7.262598	0.579462	4.322559
1	7.473072	-2.603820	-3.403703
1	7.419713	2.641893	3.806788
1	7.646277	4.122774	1.867334
1	7.643367	-4.124149	-1.922556
1	7.881850	-4.411005	0.499947
1	7.838570	4.530429	-0.239718
1	8.083358	3.585261	-2.489546
1	8.081322	-3.661903	2.496112

1	8.296884	-1.718849	4.006332
1	8.278879	1.986264	-3.896229
1	8.498613	-0.446413	-4.271027

Nanotube (7,5) u06v02
B3LYP/STO-3G Energy: -5585.795178

6	-7.741371	-3.806896	-1.071305
6	-7.621791	-3.952647	0.294547
6	-7.257577	4.301522	-1.062530
6	-7.150450	3.757027	-2.326341
6	-7.286916	-2.744202	3.034912
6	-7.113673	-1.657296	3.878334
6	-6.932218	1.361039	-4.144311
6	-6.843949	-0.011569	-4.340346
6	-6.716308	1.313197	4.221810
6	-6.540633	2.588639	3.691723
6	-6.659984	-2.718561	-3.068330
6	-6.570590	-3.514501	-1.886802
6	-6.214114	4.274173	1.230580
6	-6.095496	4.376452	-0.190585
6	-6.327765	-3.859047	0.952828
6	-6.172077	-3.302397	2.303337
6	-5.876443	3.278602	-2.835647
6	-5.776572	2.126737	-3.746111
6	-5.811301	-1.067617	4.076744
6	-5.620445	0.382827	4.283787
6	-5.593890	-0.708308	-4.181226
6	-5.513457	-2.077088	-3.601643
6	-5.256937	3.028141	3.218935
6	-5.102327	3.914288	2.030030
6	-5.275836	-3.766849	-1.304626
6	-5.158443	-3.968149	0.127925
6	-4.797683	4.229516	-0.799728
6	-4.690585	3.698628	-2.145627
6	-4.853336	-2.961602	2.765961
6	-4.674396	-1.849211	3.680108
6	-4.490400	1.514137	-3.950466
6	-4.400001	0.087357	-4.193290
6	-4.296861	0.928583	4.155826
6	-4.113162	2.271649	3.645112
6	-4.206654	-2.566877	-3.193413
6	-4.093761	-3.462448	-2.074270
6	-3.773480	4.053521	1.453565
6	-3.623745	4.270789	0.040269
6	-3.834727	-3.949926	0.728677
6	-3.682874	-3.482424	2.074441
6	-3.379311	3.306999	-2.638554
6	-3.278217	2.230972	-3.580444
6	-3.327996	-1.351074	3.931453
6	-3.139128	0.044120	4.211676
6	-3.089724	-0.556094	-4.138036
6	-2.998310	-1.917534	-3.676750
6	-2.766738	2.716176	3.294466
6	-2.599547	3.658729	2.214930
6	-2.782927	-3.776614	-1.526271
6	-2.660967	-4.067687	-0.112505
6	-2.305942	4.195820	-0.569736
6	-2.189015	3.747591	-1.943676
6	-2.357937	-3.214466	2.591509
6	-2.183387	-2.153655	3.570741
6	-1.983467	1.659353	-3.874021
6	-1.894424	0.242129	-4.196751
6	-1.809190	0.600874	4.195221
6	-1.624819	1.981402	3.762183
6	-1.707140	-2.469894	-3.346186
6	-1.603442	-3.449801	-2.275806
6	-1.284101	3.891116	1.674266

6	-1.137155	4.206681	0.262451
6	-1.355077	-4.097303	0.494776
6	-1.206266	-3.699172	1.880622
6	-0.893703	3.392576	-2.464782
6	-0.792463	2.356720	-3.471763
6	-0.858634	-1.669733	3.859505
6	-0.671756	-0.280051	4.211030
6	-0.603556	-0.404379	-4.174878
6	-0.511216	-1.788123	-3.779724
6	-0.295761	2.444701	3.436612
6	-0.123587	3.438868	2.407990
6	-0.299059	-3.776047	-1.735449
6	-0.177135	-4.144746	-0.348571
6	0.177134	4.144848	-0.347368
6	0.299059	3.776554	-1.734354
6	0.123586	-3.439569	2.406993
6	0.295761	-2.445702	3.435904
6	0.511217	1.789224	-3.779206
6	0.603557	0.405595	-4.174761
6	0.671755	0.278826	4.211110
6	0.858633	1.668609	3.859987
6	0.792464	-2.355708	-3.472446
6	0.893704	-3.391857	-2.465765
6	1.206265	3.698624	1.881695
6	1.355077	4.097159	0.495965
6	1.137154	-4.206757	0.261230
6	1.284100	-3.891604	1.673138
6	1.603442	3.450465	-2.274806
6	1.707140	2.470869	-3.345470
6	1.624818	-1.982497	3.761609
6	1.809190	-0.602095	4.195046
6	1.894425	-0.240907	-4.196820
6	1.983468	-1.658224	-3.874501
6	2.183386	2.152615	3.571363
6	2.357936	3.213710	2.592440
6	2.189015	-3.747024	-1.944763
6	2.305942	-4.195655	-0.570953
6	2.660967	4.067721	-0.111324
6	2.782927	3.777060	-1.525175
6	2.599546	-3.659376	2.213869
6	2.766737	-2.717136	3.293678
6	2.998311	1.918605	-3.676194
6	3.089725	0.557299	-4.137875
6	3.139128	-0.045346	4.211662
6	3.327995	1.349929	3.931843
6	3.278218	-2.229929	-3.581089
6	3.379311	-3.306229	-2.639512
6	3.682874	3.481818	2.075450
6	3.834727	3.949714	0.729823
6	3.623744	-4.270802	0.039030
6	3.773480	-4.053946	1.452390
6	4.093762	3.463053	-2.073265
6	4.206654	2.567808	-3.192669
6	4.113162	-2.272710	3.644453
6	4.296860	-0.929792	4.155554
6	4.400002	-0.086136	-4.193314
6	4.490402	-1.512987	-3.950903
6	4.674395	1.848139	3.680642
6	4.853335	2.960795	2.766818
6	4.690585	-3.698003	-2.146698
6	4.797683	-4.229284	-0.800955
6	5.158443	3.968113	0.129077
6	5.275837	3.767230	-1.303532
6	5.102327	-3.914881	2.028895
6	5.256937	-3.029078	3.218057
6	5.513458	2.078138	-3.601041
6	5.593892	0.709525	-4.181019
6	5.620445	-0.384074	4.283674
6	5.811300	1.066429	4.077052
6	5.776574	-2.125645	-3.746724

6	5.876444	-3.277776	-2.836596
6	6.172077	3.301724	2.304295
6	6.327765	3.858769	0.953949
6	6.095495	-4.376399	-0.191854
6	6.214113	-4.274533	1.229341
6	6.570591	3.515050	-1.885781
6	6.659985	2.719457	-3.067543
6	6.540632	-2.589713	3.690971
6	6.716307	-1.314425	4.221428
6	6.843951	0.012834	-4.340339
6	6.932220	-1.359831	-4.144700
6	7.113672	1.656165	3.878812
6	7.286915	2.743317	3.035707
6	7.150450	-3.756351	-2.327429
6	7.257576	-4.301216	-1.063778
6	7.621791	3.952562	0.295695
6	7.741371	3.807210	-1.070199
1	-8.734795	-3.770965	-1.539570
1	-8.527629	-4.037303	0.908640
1	-8.244796	4.555137	-0.651904
1	-8.059866	3.584155	-2.916214
1	-8.304755	-3.089451	2.812936
1	-7.998321	-1.165910	4.303547
1	-7.921559	1.836049	-4.147626
1	-7.767015	-0.586127	-4.491404
1	-7.733538	0.968491	4.447545
1	-7.425548	3.213200	3.513294
1	-7.660350	-2.413319	-3.401246
1	-7.226208	4.234615	1.653526
1	7.226207	-4.235096	1.652298
1	7.660346	2.414317	-3.400549
1	7.425548	-3.214224	3.512362
1	7.733537	-0.969785	4.447264
1	7.767017	0.587436	-4.491230
1	7.921561	-1.834840	-4.148149
1	7.998321	1.164655	4.303883
1	8.304755	3.088632	2.813832
1	8.059867	-3.583306	-2.917251
1	8.244794	-4.554953	-0.653228
1	8.527629	4.037042	0.909814
1	8.734797	3.771421	-1.538474

Nanotube (7,5) u06v03
B3LYP/STO-3G Energy: -5661.093292

6	7.750107	-3.609790	1.947386
6	7.600180	-4.096644	0.666964
6	7.502623	4.236104	-0.133160
6	7.401151	4.038090	1.228360
6	7.250322	-3.622781	-2.288140
6	7.095053	-2.783896	-3.379900
6	7.146225	2.196479	3.602239
6	7.022661	0.924130	4.144892
6	6.782915	0.012360	-4.468465
6	6.655135	1.385088	-4.281850
6	6.738587	-2.010713	3.609340
6	6.603631	-3.078520	2.673531
6	6.420312	3.654401	-2.332454
6	6.328242	4.120722	-0.985353
6	6.296322	-4.130699	0.020093
6	6.132003	-3.934473	-1.424685
6	6.122052	3.746047	1.854903
6	6.005371	2.870861	3.031099
6	5.806952	-2.218937	-3.709456
6	5.657226	-0.866031	-4.280098
6	5.750008	0.250092	4.182494
6	5.620163	-1.217598	3.974714
6	5.392150	1.974514	-3.927146

6	5.284114	3.139048	-3.004182
6	5.290843	-3.429911	2.190436
6	5.139924	-3.986722	0.858371
6	5.036654	4.177286	-0.347268
6	4.937187	4.012722	1.091020
6	4.815637	-3.679035	-1.945917
6	4.654084	-2.833395	-3.114348
6	4.706141	2.373009	3.399002
6	4.579874	1.060141	4.002322
6	4.353379	-0.261294	-4.287169
6	4.219471	1.173820	-4.137331
6	4.293385	-1.753803	3.721449
6	4.133593	-2.901165	2.869876
6	3.970530	3.465437	-2.471277
6	3.850983	4.040278	-1.158925
6	3.806695	-4.076583	0.287021
6	3.643647	-3.962664	-1.131150
6	3.624011	3.801540	1.679614
6	3.508645	3.007931	2.867450
6	3.319900	-2.369795	-3.471551
6	3.168929	-1.090203	-4.101382
6	3.251168	0.466398	4.127922
6	3.112727	-0.963276	4.035265
6	2.893329	1.738317	-3.900248
6	2.772489	2.928089	-3.096579
6	2.803392	-3.301457	2.434571
6	2.645186	-3.935859	1.143943
6	2.541148	4.164983	-0.537938
6	2.434568	4.086173	0.905189
6	2.316561	-3.788071	-1.685377
6	2.156609	-3.011482	-2.901957
6	2.202777	2.572486	3.310689
6	2.079510	1.291110	3.990654
6	1.855356	-0.502800	-4.218572
6	1.720604	0.946651	-4.155868
6	1.800321	-1.540972	3.874570
6	1.647940	-2.758689	3.092377
6	1.472524	3.335025	-2.622346
6	1.359250	4.002639	-1.335068
6	1.326831	-4.074350	0.579026
6	1.163808	-4.035100	-0.861671
6	1.138527	3.917854	1.511813
6	1.025301	3.179431	2.752953
6	0.842391	-2.574195	-3.294609
6	0.691636	-1.318177	-3.996570
6	0.771512	0.702735	4.151366
6	0.633201	-0.732696	4.130758
6	0.412605	1.523285	-3.951271
6	0.288369	2.751950	-3.207731
6	0.326086	-3.169743	2.669065
6	0.165755	-3.868698	1.420713
6	0.054602	4.139282	-0.717617
6	-0.054607	4.139152	0.718354
6	-0.165757	-3.868442	-1.421399
6	-0.326086	-3.169263	-2.669626
6	-0.288369	2.751374	3.208220
6	-0.412602	1.522578	3.951542
6	-0.633197	-0.731957	-4.130888
6	-0.771508	0.703477	-4.151243
6	-0.691633	-1.318893	3.996341
6	-0.842390	-2.574785	3.294156
6	-1.025302	3.179923	-2.752390
6	-1.138531	3.918122	-1.511117
6	-1.163811	-4.035251	0.860955
6	-1.326834	-4.074242	-0.579749
6	-1.359254	4.002394	1.335780
6	-1.472526	3.334550	2.622939
6	-1.647940	-2.758132	-3.092866
6	-1.800318	-1.540278	-3.874846
6	-1.720601	0.945907	4.156042

6	-1.855352	-0.503556	4.218490
6	-2.079506	1.291824	-3.990431
6	-2.202776	2.573078	-3.310237
6	-2.156609	-3.012001	2.901427
6	-2.316563	-3.788369	1.684706
6	-2.434572	4.086328	-0.904462
6	-2.541153	4.164876	0.538678
6	-2.645189	-3.935646	-1.144641
6	-2.803393	-3.301014	-2.435158
6	-2.772490	2.927529	3.097101
6	-2.893327	1.737616	3.900563
6	-3.112723	-0.962554	-4.035445
6	-3.251163	0.467136	-4.127851
6	-3.168925	-1.090939	4.101201
6	-3.319898	-2.370417	3.471139
6	-3.508645	3.008442	-2.866922
6	-3.624014	3.801833	-1.678940
6	-3.643649	-3.962857	1.130447
6	-3.806698	-4.076519	-0.287745
6	-3.850988	4.040055	1.159642
6	-3.970533	3.464983	2.471893
6	-4.133593	-2.900644	-2.870393
6	-4.293382	-1.753135	-3.721769
6	-4.219467	1.173076	4.137551
6	-4.353374	-0.262064	4.287138
6	-4.579870	1.060858	-4.002151
6	-4.706139	2.373617	-3.398595
6	-4.654083	-2.833951	3.113854
6	-4.815639	-3.679375	1.945267
6	-4.937191	4.012903	-1.090309
6	-5.036659	4.177203	0.348008
6	-5.139927	-3.986552	-0.859078
6	-5.290845	-3.429507	-2.191046
6	-5.284116	3.138497	3.004743
6	-5.392148	1.973806	3.927507
6	-5.620160	-1.216885	-3.974945
6	-5.750003	0.250842	-4.182474
6	-5.657222	-0.866800	4.279966
6	-5.806949	-2.219602	3.709078
6	-6.005369	2.871401	-3.030604
6	-6.122055	3.746366	-1.854244
6	-6.132005	-3.934714	1.423988
6	-6.296326	-4.130675	-0.020826
6	-6.328247	4.120519	0.986082
6	-6.420316	3.653961	2.333102
6	-6.603631	-3.078028	-2.674080
6	-6.738585	-2.010060	-3.609707
6	-6.655132	1.384318	4.282117
6	-6.782909	0.011558	4.468494
6	-7.022656	0.924877	-4.144764
6	-7.146222	2.197127	-3.601877
6	-7.095050	-2.784500	3.379421
6	-7.250323	-3.623179	2.287503
6	-7.401155	4.038286	-1.227647
6	-7.502628	4.236048	0.133910
6	-7.600183	-4.096497	-0.667690
6	-7.750110	-3.609418	-1.948027
1	8.752686	-3.489498	2.380801
1	8.490792	-4.367961	0.085592
1	8.489365	4.345864	-0.604110
1	8.314611	3.995374	1.835486
1	8.260464	-3.937238	-1.996365
1	7.985599	-2.450811	-3.928398
1	8.148268	2.625594	3.474870
1	7.931218	0.378456	4.430842
1	7.784842	-0.413298	-4.608314
1	7.560938	2.005198	-4.278372
1	7.753189	-1.662934	3.842154
1	7.423291	3.475349	-2.740656
1	-7.423294	3.474833	2.741272

1	-7.753187	-1.662236	-3.842456
1	-7.560934	2.004429	4.278752
1	-7.784835	-0.414125	4.608275
1	-7.931211	0.379259	-4.430825
1	-8.148264	2.626220	-3.474437
1	-7.985595	-2.451518	3.927983
1	-8.260468	-3.937578	1.995668
1	-8.314614	3.995677	-1.834781
1	-8.489372	4.345716	0.604879
1	-8.490797	-4.367910	-0.086365
1	-8.752688	-3.489041	-2.381418

Nanotube (7,5) u06v04
B3LYP/STO-3G Energy: -5736.390888

6	7.884570	2.820207	-2.919416
6	7.775234	3.622146	-1.804911
6	7.517643	-4.220433	1.105985
6	7.385955	-4.374553	-0.257906
6	7.483953	3.930723	1.178460
6	7.336418	3.404080	2.450680
6	7.111742	-3.196744	-3.019603
6	7.003258	-2.103936	-3.868026
6	6.992069	0.989485	4.225624
6	6.831794	-0.380755	4.400709
6	6.798517	0.877081	-4.097083
6	6.709476	2.151132	-3.465450
6	6.502982	-3.066364	3.102439
6	6.367349	-3.858556	1.922780
6	6.487082	3.855536	-1.165665
6	6.352127	4.039451	0.282302
6	6.097213	-4.216706	-0.914403
6	5.970035	-3.669435	-2.271922
6	6.043993	2.975420	2.935961
6	5.879925	1.819278	3.837226
6	5.744484	-1.425832	-4.053664
6	5.652916	0.047743	-4.228287
6	5.548092	-1.008556	4.232527
6	5.393791	-2.367233	3.642281
6	5.415924	2.651873	-3.067683
6	5.308446	3.534727	-1.920323
6	5.058890	-4.042965	1.345287
6	4.926354	-4.248030	-0.085371
6	5.042803	3.961289	0.874238
6	4.890771	3.446998	2.223288
6	4.673223	-3.246712	-2.731317
6	4.561478	-2.129548	-3.650242
6	4.564508	1.271012	4.023363
6	4.397786	-0.150557	4.251283
6	4.345676	0.668178	-4.100287
6	4.232099	1.999933	-3.569702
6	4.061812	-2.785691	3.236671
6	3.897685	-3.672817	2.117421
6	3.991703	3.803394	-1.368271
6	3.859114	4.057981	0.034381
6	3.604109	-4.156603	-0.683344
6	3.476228	-3.688837	-2.031197
6	3.555995	3.124191	2.709710
6	3.393397	2.054182	3.649947
6	3.244228	-1.550138	-3.899185
6	3.140208	-0.143586	-4.177538
6	3.055005	-0.722409	4.191772
6	2.890260	-2.074723	3.725720
6	2.921510	2.535094	-3.228720
6	2.807343	3.480132	-2.141641
6	2.569750	-3.916771	1.573518
6	2.427772	-4.202089	0.161500
6	2.540705	4.064432	0.637500

6	2.392756	3.628141	2.013835
6	2.168142	-3.342742	-2.545675
6	2.056545	-2.278270	-3.529874
6	2.070362	1.550984	3.937708
6	1.904552	0.139055	4.255520
6	1.844086	0.493312	-4.150370
6	1.738057	1.874660	-3.707512
6	1.570818	-2.557329	3.398778
6	1.411409	-3.529106	2.327705
6	1.504981	3.794743	-1.608859
6	1.374964	4.125679	-0.202021
6	1.120072	-4.157701	-0.442585
6	0.991703	-3.753906	-1.828787
6	1.079119	3.340212	2.528001
6	0.918913	2.310913	3.532602
6	0.759081	-1.715123	-3.814934
6	0.653543	-0.319751	-4.168524
6	0.581299	-0.436928	4.232169
6	0.414238	-1.812962	3.836064
6	0.436980	2.418065	-3.383210
6	0.321880	3.415406	-2.350931
6	0.090502	-3.785013	1.791449
6	-0.055791	-4.140389	0.404315
6	0.055792	4.140404	0.404160
6	-0.090501	3.785081	1.791307
6	-0.321879	-3.415496	-2.350803
6	-0.436980	-2.418194	-3.383119
6	-0.414240	1.813107	3.835995
6	-0.581302	0.437088	4.232151
6	-0.653544	0.319593	-4.168535
6	-0.759082	1.714978	-3.814998
6	-0.918914	-2.310779	3.532688
6	-1.079119	-3.340117	2.528126
6	-0.991701	3.753838	-1.828928
6	-1.120070	4.157686	-0.442742
6	-1.374962	-4.125689	-0.201867
6	-1.504980	-3.794806	-1.608717
6	-1.411409	3.529195	2.327572
6	-1.570819	2.557458	3.398680
6	-1.738057	-1.874801	-3.707441
6	-1.844087	-0.493469	-4.150350
6	-1.904555	-0.138894	4.255522
6	-2.070365	-1.550835	3.937764
6	-2.056545	2.278137	-3.529958
6	-2.168141	3.342646	-2.545801
6	-2.392756	-3.628067	2.013970
6	-2.540704	-4.064411	0.637652
6	-2.427770	4.202099	0.161341
6	-2.569749	3.916834	1.573369
6	-2.807342	-3.480217	-2.141512
6	-2.921509	-2.535219	-3.228625
6	-2.890262	2.074865	3.725638
6	-3.055008	0.722567	4.191740
6	-3.140209	0.143428	-4.177540
6	-3.244228	1.549989	-3.899240
6	-3.393399	-2.054044	3.650020
6	-3.555995	-3.124090	2.709825
6	-3.476227	3.688763	-2.031336
6	-3.604107	4.156583	-0.683501
6	-3.859113	-4.057986	0.034532
6	-3.991701	-3.803451	-1.368130
6	-3.897684	3.672901	2.117281
6	-4.061812	2.785814	3.236562
6	-4.232099	-2.000070	-3.569626
6	-4.345678	-0.668334	-4.100258
6	-4.397789	0.150718	4.251270
6	-4.564511	-1.270859	4.023404
6	-4.561478	2.129410	-3.650317
6	-4.673223	3.246610	-2.731437
6	-4.890770	-3.446918	2.223414

6	-5.042801	-3.961263	0.874385
6	-4.926351	4.248034	-0.085532
6	-5.058889	4.043024	1.345133
6	-5.308445	-3.534806	-1.920192
6	-5.415924	-2.651994	-3.067584
6	-5.393792	2.367374	3.642188
6	-5.548095	1.008717	4.232482
6	-5.652917	-0.047904	-4.228277
6	-5.744485	1.425677	-4.053709
6	-5.879927	-1.819133	3.837286
6	-6.043993	-2.975312	2.936067
6	-5.970034	3.669354	-2.272059
6	-6.097211	4.216681	-0.914562
6	-6.352125	-4.039450	0.282451
6	-6.487080	-3.855590	-1.165522
6	-6.367348	3.858639	1.922634
6	-6.502980	3.066494	3.102326
6	-6.709476	-2.151266	-3.465365
6	-6.798519	-0.877233	-4.097035
6	-6.831797	0.380922	4.400684
6	-6.992073	-0.989324	4.225647
6	-7.003259	2.103787	-3.868093
6	-7.111741	3.196631	-3.019717
6	-7.336417	-3.403992	2.450803
6	-7.483951	-3.930687	1.178604
6	-7.385952	4.374556	-0.258071
6	-7.517642	4.220486	1.105826
6	-7.775232	-3.622223	-1.804774
6	-7.884570	-2.820319	-2.919305
1	8.873666	2.566603	-3.325416
1	8.684554	4.010390	-1.328241
1	8.513143	-4.234221	1.571018
1	8.284026	-4.515079	-0.873170
1	8.493111	4.135326	0.798924
1	8.231788	3.201071	3.052308
1	8.106251	-3.608832	-2.806225
1	7.915691	-1.676616	-4.303767
1	8.005346	1.411104	4.234239
1	7.723978	-1.004546	4.541776
1	7.798970	0.452731	-4.250521
1	7.519218	-2.815229	3.432483
1	-7.519202	2.815397	3.432395
1	-7.798986	-0.452875	-4.250458
1	-7.723981	1.004717	4.541727
1	-8.005353	-1.410942	4.234267
1	-7.915693	1.676447	-4.303813
1	-8.106251	3.608726	-2.806353
1	-8.231789	-3.200960	3.052422
1	-8.493110	-4.135304	0.799075
1	-8.284023	4.515061	-0.873341
1	-8.513143	4.234288	1.570858
1	-8.684552	-4.010450	-1.328090
1	-8.873670	-2.566720	-3.325307

Nanotube (7,5) u06v05
B3LYP/STO-3G Energy: -5811.688012

6	-8.023447	-2.113178	-3.405073
6	-7.872966	-3.171323	-2.537117
6	-7.656003	3.669440	2.284928
6	-7.562348	4.170249	1.004308
6	-7.496102	-4.228192	0.260599
6	-7.321207	-4.041259	1.620694
6	-7.342169	3.743039	-1.972434
6	-7.239146	2.906759	-3.074065
6	-6.964809	-2.155122	3.947330
6	-6.821463	-0.873365	4.464870
6	-6.996684	0.089717	-4.065246

6	-6.872696	-1.301139	-3.785968
6	-6.570884	2.062364	3.893908
6	-6.478919	3.133455	2.956614
6	-6.564334	-3.534202	-2.007631
6	-6.387311	-4.079451	-0.659779
6	-6.288443	4.212302	0.301046
6	-6.187993	4.032804	-1.152470
6	-6.021633	-3.722138	2.169984
6	-5.850231	-2.832488	3.332363
6	-5.974672	2.325341	-3.454124
6	-5.866313	0.948860	-4.003411
6	-5.551925	-0.194587	4.434775
6	-5.435615	1.272371	4.212075
6	-5.561761	-1.860950	-3.560284
6	-5.411086	-3.007151	-2.681994
6	-5.188694	3.489744	2.418572
6	-5.096806	4.057062	1.085763
6	-5.063407	-4.128866	-0.097560
6	-4.881476	-3.972273	1.334531
6	-4.897062	3.769836	-1.732595
6	-4.792414	2.927011	-2.909332
6	-4.538747	-2.321543	3.623342
6	-4.388314	-1.002635	4.206270
6	-4.547691	0.343581	-4.068312
6	-4.401311	-1.077446	-3.902741
6	-4.122371	1.811511	3.900718
6	-4.002283	2.960403	3.044815
6	-4.076846	-3.381796	-2.247790
6	-3.902479	-3.983398	-0.960915
6	-3.789884	4.149902	0.456220
6	-3.689639	4.043469	-0.968237
6	-3.539149	-3.753749	1.856007
6	-3.366850	-2.955460	3.033178
6	-3.473528	2.457240	-3.325380
6	-3.356158	1.172610	-3.958140
6	-3.057208	-0.404421	4.264905
6	-2.926693	1.024037	4.162651
6	-3.074341	-1.655534	-3.740721
6	-2.917823	-2.846309	-2.939131
6	-2.692925	3.365394	2.553391
6	-2.592260	4.004002	1.260253
6	-2.567243	-4.115965	-0.409467
6	-2.387142	-4.039192	1.027043
6	-2.389018	3.866827	-1.581480
6	-2.286845	3.091115	-2.806252
6	-2.042758	-2.511793	3.408503
6	-1.890444	-1.227720	4.075742
6	-2.050044	0.577121	-4.124502
6	-1.912911	-0.869344	-4.058307
6	-1.623058	1.605452	3.944773
6	-1.508057	2.824090	3.159461
6	-1.597490	-3.262773	-2.536671
6	-1.424226	-3.940860	-1.264763
6	-1.299517	4.145008	0.637457
6	-1.201209	4.108270	-0.808977
6	-1.063746	-3.862934	1.566334
6	-0.891266	-3.117347	2.795761
6	-0.989108	2.646616	-3.253362
6	-0.872396	1.391133	-3.956719
6	-0.578160	-0.635724	4.173999
6	-0.443649	0.800448	4.148713
6	-0.596934	-1.451874	-3.915487
6	-0.440758	-2.680883	-3.181593
6	-0.206958	3.240134	2.680308
6	-0.103207	3.940146	1.426745
6	-0.090159	-4.083296	-0.713364
6	0.090159	-4.083248	0.713644
6	0.103202	3.940049	-1.427022
6	0.206955	3.239952	-2.680534
6	0.440760	-2.680664	3.181775

6	0.596937	-1.451607	3.915585
6	0.443652	0.800165	-4.148769
6	0.578164	-0.636009	-4.173955
6	0.872398	1.391404	3.956619
6	0.989107	2.646839	3.253175
6	0.891267	-3.117540	-2.795548
6	1.063745	-3.863043	-1.566070
6	1.201202	4.108328	0.808690
6	1.299511	4.144970	-0.637746
6	1.424226	-3.940773	1.265032
6	1.597492	-3.262598	2.536893
6	1.508057	2.823878	-3.159658
6	1.623061	1.605184	-3.944883
6	1.912915	-0.869065	4.058362
6	2.050046	0.577405	4.124457
6	1.890447	-1.227999	-4.075656
6	2.042759	-2.512027	-3.408330
6	2.286841	3.091311	2.806033
6	2.389013	3.866940	1.581209
6	2.387141	-4.039265	-1.026767
6	2.567243	-4.115939	0.409749
6	2.592254	4.003926	-1.260533
6	2.692923	3.365226	-2.553626
6	2.917825	-2.846107	2.939321
6	3.074344	-1.655274	3.740829
6	2.926697	1.023753	-4.162714
6	3.057212	-0.404712	-4.264871
6	3.356160	1.172884	3.958048
6	3.473525	2.457473	3.325204
6	3.366850	-2.955671	-3.032975
6	3.539147	-3.753884	-1.855752
6	3.689630	4.043548	0.967955
6	3.789878	4.149884	-0.456510
6	3.902479	-3.983335	0.961187
6	4.076847	-3.381640	2.248017
6	4.002285	2.960201	-3.045013
6	4.122376	1.811242	-3.900828
6	4.401315	-1.077174	3.902801
6	4.547694	0.343866	4.068277
6	4.388316	-1.002924	-4.206194
6	4.538747	-2.321797	-3.623183
6	4.792409	2.927219	2.909125
6	4.897055	3.769967	1.732332
6	4.881474	-3.972372	-1.334261
6	5.063406	-4.128864	0.097841
6	5.096800	4.057006	-1.086042
6	5.188695	3.489587	-2.418807
6	5.411087	-3.006965	2.682194
6	5.561764	-1.860702	3.560402
6	5.435621	1.272078	-4.212135
6	5.551927	-0.194893	-4.434743
6	5.866316	0.949139	4.003331
6	5.974670	2.325591	3.453959
6	5.850230	-2.832727	-3.332171
6	6.021631	-3.722301	-2.169737
6	6.187985	4.032906	1.152193
6	6.288437	4.212301	-0.301336
6	6.387310	-4.079413	0.660059
6	6.564335	-3.534069	2.007871
6	6.478924	3.133252	-2.956809
6	6.570896	2.062072	-3.893993
6	6.872699	-1.300875	3.786047
6	6.996687	0.089999	4.065220
6	6.821467	-0.873669	-4.464782
6	6.964809	-2.155400	-3.947179
6	7.239144	2.906996	3.073866
6	7.342162	3.743205	1.972179
6	7.321205	-4.041395	-1.620428
6	7.496100	-4.228235	-0.260310
6	7.562343	4.170195	-1.004588

6	7.656006	3.669278	-2.285154
6	7.872967	-3.171156	2.537334
6	8.023449	-2.112945	3.405215
1	-9.026637	-1.785243	-3.711409
1	-8.763394	-3.688814	-2.157228
1	-8.638977	3.544576	2.760278
1	-8.478026	4.446776	0.465712
1	-8.512108	-4.352432	-0.135932
1	-8.202211	-4.020098	2.275280
1	-8.336854	4.066204	-1.639307
1	-8.155749	2.586624	-3.586553
1	-7.970598	-2.588237	3.870951
1	-7.718592	-0.326798	4.783826
1	-8.007211	0.518414	-4.083241
1	-7.574086	1.712804	4.171137
1	7.574155	1.712447	-4.171163
1	8.007232	0.518701	4.083198
1	7.718598	-0.327112	-4.783755
1	7.970593	-2.588514	-3.870788
1	8.155739	2.586909	3.586382
1	8.336828	4.066365	1.639046
1	8.202201	-4.020290	-2.275018
1	8.512088	-4.352468	0.136225
1	8.478022	4.446756	-0.466006
1	8.639002	3.544344	-2.760485
1	8.763394	-3.688680	2.157487
1	9.026637	-1.784988	3.711530

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B3LYP/STO-3G Energy: -5886.984712

6	8.038454	1.080366	-4.001792
6	7.921697	2.327028	-3.430519
6	7.803582	-3.039236	2.982182
6	7.669817	-3.850667	1.876894
6	7.634790	4.071572	-0.988492
6	7.497740	4.242566	0.377345
6	7.362409	-4.202198	-1.102300
6	7.230520	-3.675463	-2.377627
6	7.194232	3.022886	3.119233
6	7.057182	1.918890	3.950726
6	6.976275	-1.202191	-4.047518
6	6.870477	0.213986	-4.129857
6	6.773535	-1.061002	4.153755
6	6.648780	-2.334384	3.526016
6	6.631309	2.832740	-2.976429
6	6.498048	3.707519	-1.811236
6	6.374447	-4.057056	1.243516
6	6.231447	-4.255848	-0.202572
6	6.211153	4.093917	1.024011
6	6.066642	3.534775	2.378495
6	5.957651	-3.192169	-2.858094
6	5.841181	-2.001320	-3.737000
6	5.782297	1.270933	4.126645
6	5.651177	-0.201720	4.289904
6	5.570273	0.832332	-4.020568
6	5.454341	2.167793	-3.463218
6	5.341167	-2.802097	3.134294
6	5.207358	-3.692360	1.995517
6	5.191102	3.921122	-1.246686
6	5.049389	4.139809	0.182131
6	4.925009	-4.134962	-0.795028
6	4.789152	-3.619295	-2.145197
6	4.760489	3.133330	2.824465
6	4.618075	2.008840	3.729072
6	4.525943	-1.413888	-3.917920
6	4.394774	0.004574	-4.118403
6	4.327215	-0.786066	4.162557

6	4.176561	-2.115043	3.634882
6	4.137010	2.661819	-3.105549
6	4.005214	3.576776	-2.012999
6	3.882473	-3.928327	1.447338
6	3.740382	-4.188508	0.046992
6	3.721462	4.080635	0.776752
6	3.577080	3.610691	2.121818
6	3.461419	-3.251285	-2.629087
6	3.332739	-2.169223	-3.563622
6	3.285537	1.462115	3.971383
6	3.143583	0.057896	4.242793
6	3.077438	0.624401	-4.072764
6	2.953670	1.982551	-3.603540
6	2.850959	-2.616679	3.299793
6	2.709169	-3.565972	2.219929
6	2.686998	3.866542	-1.479132
6	2.547691	4.161572	-0.068310
6	2.421906	-4.157848	-0.555059
6	2.286221	-3.716719	-1.931591
6	2.260020	3.294408	2.631353
6	2.118308	2.225026	3.606961
6	2.024856	-1.616309	-3.838533
6	1.899960	-0.200727	-4.143382
6	1.830491	-0.543293	4.216155
6	1.686516	-1.922289	3.777055
6	1.648088	2.510139	-3.288835
6	1.517728	3.496460	-2.231945
6	1.398090	-3.849076	1.691254
6	1.256704	-4.183334	0.286460
6	1.238504	4.148745	0.532322
6	1.096186	3.740837	1.915277
6	0.978039	-3.382653	-2.439509
6	0.847715	-2.343298	-3.434636
6	0.806013	1.694878	3.886675
6	0.662287	0.301877	4.235001
6	0.593969	0.418492	-4.120563
6	0.468786	1.799538	-3.729362
6	0.370703	-2.432252	3.457505
6	0.227107	-3.432764	2.432731
6	0.202335	3.797034	-1.701775
6	0.063604	4.162612	-0.317730
6	-0.063606	-4.162633	-0.317494
6	-0.202336	-3.797134	-1.701560
6	-0.227109	3.432901	2.432537
6	-0.370703	2.432447	3.457367
6	-0.468784	-1.799753	-3.729262
6	-0.593967	-0.418729	-4.120541
6	-0.662285	-0.301638	4.235018
6	-0.806012	-1.694658	3.886771
6	-0.847713	2.343099	-3.434769
6	-0.978039	3.382510	-2.439701
6	-1.096188	-3.740728	1.915489
6	-1.238507	-4.148715	0.532556
6	-1.256706	4.183347	0.286221
6	-1.398091	3.849169	1.691035
6	-1.517728	-3.496588	-2.231748
6	-1.648087	-2.510329	-3.288696
6	-1.686515	1.922502	3.776947
6	-1.830489	0.543531	4.216126
6	-1.899957	0.200489	-4.143399
6	-2.024854	1.616088	-3.838628
6	-2.118309	-2.224821	3.607088
6	-2.260023	-3.294256	2.631539
6	-2.286221	3.716604	-1.931804
6	-2.421908	4.157811	-0.555297
6	-2.547694	-4.161573	-0.068075
6	-2.687000	-3.866626	-1.478914
6	-2.709169	3.566094	2.219726
6	-2.850958	2.616864	3.299645
6	-2.953668	-1.982758	-3.603434

6	-3.077436	-0.624635	-4.072737
6	-3.143581	-0.057655	4.242801
6	-3.285537	-1.461889	3.971469
6	-3.332737	2.169018	-3.563749
6	-3.461419	3.251131	-2.629274
6	-3.577083	-3.610564	2.122021
6	-3.721466	-4.080584	0.776981
6	-3.740383	4.188503	0.046752
6	-3.882474	3.928403	1.447113
6	-4.005216	-3.576888	-2.012800
6	-4.137009	-2.661996	-3.105405
6	-4.176559	2.115249	3.634767
6	-4.327211	0.786304	4.162523
6	-4.394772	-0.004809	-4.118413
6	-4.525941	1.413663	-3.918008
6	-4.618076	-2.008625	3.729190
6	-4.760492	-3.133163	2.824643
6	-4.789152	3.619167	-2.145405
6	-4.925011	4.134908	-0.795264
6	-5.049393	-4.139789	0.182363
6	-5.191105	-3.921187	-1.246467
6	-5.207358	3.692468	1.995308
6	-5.341164	2.802276	3.134142
6	-5.454340	-2.167990	-3.463105
6	-5.570271	-0.832561	-4.020532
6	-5.651174	0.201968	4.289913
6	-5.782297	-1.270695	4.126729
6	-5.841179	2.001106	-3.737121
6	-5.957650	3.192003	-2.858280
6	-6.066645	-3.534630	2.378695
6	-6.211158	-4.093846	1.024241
6	-6.231449	4.255826	-0.202815
6	-6.374447	4.057119	1.243286
6	-6.498050	-3.707614	-1.811030
6	-6.631309	-2.832906	-2.976276
6	-6.648775	2.334591	3.525901
6	-6.773528	1.061251	4.153729
6	-6.870475	-0.214220	-4.129859
6	-6.976274	1.201961	-4.047595
6	-7.057182	-1.918665	3.950852
6	-7.194233	-3.022704	3.119413
6	-7.230520	3.675321	-2.377840
6	-7.362411	4.202122	-1.102539
6	-7.497745	-4.242525	0.377582
6	-7.634794	-4.071610	-0.988265
6	-7.669817	3.850768	1.876681
6	-7.803578	3.039409	2.982022
6	-7.921696	-2.327221	-3.430398
6	-8.038452	-1.080593	-4.001748
1	9.029136	0.670165	-4.242087
1	8.826393	2.912148	-3.220786
1	8.800444	-2.807917	3.382508
1	8.567414	-4.267394	1.402012
1	8.639418	4.075770	-1.430207
1	8.396452	4.378157	0.992776
1	8.364306	-4.445536	-0.726114
1	8.132016	-3.512190	-2.982253
1	8.199522	3.411034	2.911153
1	7.958635	1.461433	4.378591
1	7.981947	-1.636799	-3.983429
1	7.785363	-0.663699	4.304601
1	-7.785362	0.663955	4.304594
1	-7.981943	1.636574	-3.983538
1	-7.958633	-1.461193	4.378701
1	-8.199520	-3.410866	2.911359
1	-8.132015	3.512016	-2.982458
1	-8.364311	4.445471	-0.726364
1	-8.396458	-4.378075	0.993020
1	-8.639423	-4.075824	-1.429980
1	-8.567414	4.267468	1.401774

1	-8.800440	2.808120	3.382367
1	-8.826393	-2.912327	-3.220629
1	-9.029131	-0.670406	-4.242071

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B3LYP/STO-3G Energy: -5962.280995

6	8.252134	0.058798	-3.971468
6	8.121009	1.408912	-3.742297
6	7.820482	-2.134527	3.829892
6	7.718334	-3.202486	2.966527
6	7.770561	3.717697	-1.835607
6	7.596635	4.231478	-0.563862
6	7.495506	-4.306662	0.168472
6	7.398959	-4.125255	-1.201561
6	7.214156	3.754029	2.390238
6	7.051328	2.899792	3.472051
6	7.190364	-2.165194	-3.456232
6	7.087085	-0.819350	-3.901544
6	6.758017	0.070833	4.424164
6	6.650460	-1.320477	4.141203
6	6.818708	2.006083	-3.465490
6	6.655312	3.148736	-2.568352
6	6.441002	-3.573126	2.370595
6	6.339128	-4.136481	1.021790
6	6.291534	4.247242	0.064448
6	6.108212	4.053136	1.511329
6	6.138857	-3.790559	-1.824149
6	6.046210	-2.866043	-2.980665
6	5.769817	2.310856	3.772196
6	5.631919	0.929575	4.303242
6	5.784227	-0.201813	-3.988614
6	5.654413	1.231315	-3.796324
6	5.353858	-1.882349	3.846666
6	5.252608	-3.036601	2.972268
6	5.333784	3.494182	-2.113524
6	5.153549	4.071919	-0.792893
6	5.049557	-4.183142	0.383026
6	4.951275	-4.031241	-1.057658
6	4.789251	3.773632	2.009570
6	4.618801	2.916498	3.167380
6	4.736883	-2.353430	-3.340790
6	4.611649	-1.034058	-3.900952
6	4.312163	0.323586	4.292443
6	4.175998	-1.097716	4.120161
6	4.328835	1.792613	-3.611933
6	4.168944	2.957446	-2.796342
6	3.944499	-3.415697	2.467420
6	3.842343	-4.028306	1.178041
6	3.810169	4.160890	-0.239354
6	3.627547	4.049593	1.175903
6	3.637759	-3.808086	-1.654706
6	3.534378	-3.000840	-2.836047
6	3.279260	2.440609	3.502093
6	3.127537	1.152164	4.117470
6	3.293459	-0.431298	-4.048528
6	3.158038	1.000161	-3.947876
6	2.860284	-1.677532	3.886949
6	2.749194	-2.873745	3.087487
6	2.836572	3.368004	-2.390566
6	2.659435	4.016700	-1.109237
6	2.540653	-4.163350	0.552528
6	2.443025	-4.089565	-0.892483
6	2.295008	3.867331	1.713069
6	2.123002	3.079907	2.922069
6	2.233488	-2.544759	-3.277026
6	2.117293	-1.254692	-3.935653
6	1.813831	0.555273	4.206739

6	1.681633	-0.890374	4.134506
6	1.844649	1.583418	-3.814433
6	1.687313	2.809599	-3.053310
6	1.452909	-3.295379	2.615068
6	1.351784	-3.982799	1.341414
6	1.334607	4.155074	-0.561895
6	1.152883	4.114634	0.875717
6	1.149171	-3.906742	-1.503969
6	1.046320	-3.153709	-2.733600
6	0.802386	2.630855	3.289318
6	0.646744	1.369441	3.974883
6	0.811765	-0.658482	-4.105472
6	0.677113	0.776229	-4.085944
6	0.376209	-1.475074	3.921186
6	0.261673	-2.710403	3.189826
6	0.359280	3.230462	-2.654490
6	0.183952	3.942852	-1.417842
6	0.049981	-4.129312	0.717225
6	-0.049981	-4.129339	-0.717062
6	-0.183955	3.942907	1.417688
6	-0.359282	3.230566	2.654364
6	-0.261671	-2.710527	-3.189719
6	-0.376207	-1.475226	-3.921128
6	-0.677111	0.776389	4.085915
6	-0.811764	-0.658322	4.105500
6	-0.646743	1.369286	-3.974938
6	-0.802387	2.630726	-3.289422
6	-1.046319	-3.153602	2.733725
6	-1.149172	-3.906683	1.504123
6	-1.152886	4.114598	-0.875878
6	-1.334610	4.155095	0.561733
6	-1.351784	-3.982850	-1.341258
6	-1.452908	-3.295480	-2.614939
6	-1.687314	2.809717	3.053201
6	-1.844648	1.583566	3.814373
6	-1.681631	-0.890536	-4.134473
6	-1.813829	0.555108	-4.206763
6	-2.117291	-1.254539	3.935705
6	-2.233487	-2.544631	3.277128
6	-2.123003	3.079791	-2.922190
6	-2.295010	3.867261	-1.713220
6	-2.443026	-4.089528	0.892643
6	-2.540653	-4.163368	-0.552365
6	-2.659437	4.016740	1.109081
6	-2.836573	3.368096	2.390435
6	-2.749192	-2.873864	-3.087377
6	-2.860282	-1.677684	-3.886887
6	-3.158037	1.000316	3.947840
6	-3.293457	-0.431140	4.048549
6	-3.127536	1.152002	-4.117519
6	-3.279261	2.440470	-3.502190
6	-3.534377	-3.000728	2.836166
6	-3.637760	-3.808018	1.654856
6	-3.627550	4.049542	-1.176060
6	-3.810172	4.160894	0.239191
6	-3.842343	-4.028347	-1.177884
6	-3.944497	-3.415791	-2.467289
6	-4.168945	2.957553	2.796228
6	-4.328835	1.792754	3.611867
6	-4.175995	-1.097878	-4.120125
6	-4.312162	0.323417	-4.292463
6	-4.611647	-1.033905	3.900999
6	-4.736881	-2.353299	3.340886
6	-4.618803	2.916370	-3.167495
6	-4.789255	3.773547	-2.009717
6	-4.951276	-4.031193	1.057815
6	-5.049557	-4.183149	-0.382864
6	-5.153552	4.071945	0.792734
6	-5.333786	3.494261	2.113389
6	-5.252605	-3.036717	-2.972155

6	-5.353855	-1.882501	-3.846600
6	-5.654412	1.231463	3.796281
6	-5.784226	-0.201657	3.988631
6	-5.631919	0.929405	-4.303284
6	-5.769817	2.310706	-3.772291
6	-6.046209	-2.865926	2.980785
6	-6.138857	-3.790479	1.824298
6	-6.108217	4.053069	-1.511487
6	-6.291537	4.247231	-0.064613
6	-6.339128	-4.136516	-1.021631
6	-6.441000	-3.573219	-2.370462
6	-6.655314	3.148834	2.568232
6	-6.818708	2.006218	3.465418
6	-6.650458	-1.320641	-4.141161
6	-6.758018	0.070658	-4.424169
6	-7.087083	-0.819199	3.901591
6	-7.190361	-2.165060	3.456332
6	-7.051327	2.899658	-3.472173
6	-7.214158	3.753930	-2.390388
6	-7.398960	-4.125192	1.201718
6	-7.495504	-4.306661	-0.168306
6	-7.596639	4.231490	0.563697
6	-7.770564	3.717761	1.835464
6	-7.718330	-3.202608	-2.966416
6	-7.820478	-2.134684	-3.829824
6	-8.121008	1.409058	3.742252
6	-8.252132	0.058953	3.971476
1	9.248355	-0.393235	-4.074675
1	9.019795	2.034651	-3.668220
1	8.805162	-1.802024	4.186665
1	8.628661	-3.722043	2.640571
1	8.786675	3.614450	-2.237196
1	8.478061	4.525581	0.020480
1	8.486363	-4.439104	0.621550
1	8.316507	-4.116748	-1.804072
1	8.225386	4.082931	2.118367
1	7.938831	2.573188	4.029435
1	8.193597	-2.562920	-3.257226
1	7.765086	0.500656	4.497422
1	-7.765087	0.500480	-4.497437
1	-8.193610	-2.562793	3.257329
1	-7.938829	2.573042	-4.029555
1	-8.225393	4.082843	-2.118530
1	-8.316510	-4.116650	1.804226
1	-8.486359	-4.439126	-0.621376
1	-8.478065	4.525567	-0.020658
1	-8.786677	3.614526	2.237055
1	-8.628657	-3.722155	-2.640443
1	-8.805157	-1.802197	-4.186613
1	-9.019795	2.034794	3.668150
1	-9.248355	-0.393078	4.074697

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B3LYP/STO-3G Energy: -6037.576935

6	8.245466	-4.038720	0.949804
6	8.109010	-4.158126	-0.413399
6	8.039837	4.077422	1.080315
6	7.923619	3.518640	2.332978
6	7.792983	-2.893748	-3.131679
6	7.650496	-1.791180	-3.952618
6	7.637900	1.100644	4.113327
6	7.504231	-0.266534	4.287591
6	7.352669	1.197275	-4.244008
6	7.224974	2.464756	-3.694539
6	7.217929	-2.941185	2.969202
6	7.090289	-3.711330	1.782715
6	6.976646	4.116009	-1.202887

6	6.871784	4.200289	0.213557
6	6.809451	-4.003411	-1.060138
6	6.661853	-3.424048	-2.392651
6	6.633755	3.070210	2.844137
6	6.501871	1.914161	3.732951
6	6.362588	-1.149938	-4.127605
6	6.220534	0.301918	-4.309440
6	6.224413	-0.919321	4.125870
6	6.092623	-2.269585	3.527986
6	5.955190	2.941150	-3.201868
6	5.840914	3.809850	-2.002439
6	5.779589	-3.915551	1.209492
6	5.642562	-4.091612	-0.224868
6	5.571814	4.093779	0.832927
6	5.456899	3.546763	2.172691
6	5.350380	-3.035102	-2.842623
6	5.202484	-1.901904	-3.739641
6	5.196613	1.344490	3.944895
6	5.059671	-0.084203	4.167034
6	4.917447	0.892325	-4.168509
6	4.784320	2.234980	-3.634804
6	4.770045	-2.712081	3.127259
6	4.617541	-3.585534	1.993656
6	4.526171	3.989659	-1.413145
6	4.395914	4.188746	0.005380
6	4.318310	-4.017373	-0.812918
6	4.171738	-3.522789	-2.147744
6	4.139616	3.190809	2.669430
6	4.009396	2.105566	3.592782
6	3.874860	-1.351722	-3.967786
6	3.732073	0.049041	-4.222937
6	3.729508	-0.682015	4.106686
6	3.587601	-2.025495	3.627370
6	3.457920	2.716433	-3.259173
6	3.331371	3.641200	-2.169451
6	3.290371	-3.841916	1.449541
6	3.145062	-4.103529	0.040993
6	3.078513	4.145169	0.626278
6	2.955812	3.682293	1.986609
6	2.847565	-3.196101	-2.647347
6	2.701107	-2.122330	-3.603710
6	2.692469	1.571315	3.886212
6	2.556719	0.160240	4.187194
6	2.415274	0.652623	-4.184707
6	2.281318	2.024949	-3.731276
6	2.270438	-2.531980	3.301693
6	2.124125	-3.490401	2.220613
6	2.023813	3.914671	-1.614107
6	1.900293	4.215156	-0.197619
6	1.829814	-4.083608	-0.555554
6	1.683739	-3.658759	-1.935551
6	1.650843	3.369290	2.516907
6	1.522712	2.319371	3.510483
6	1.390280	-1.592078	-3.880605
6	1.248719	-0.187919	-4.212227
6	1.246484	-0.442019	4.172725
6	1.104288	-1.820549	3.758679
6	0.974173	2.531280	-3.391243
6	0.845836	3.517111	-2.342897
6	0.809264	-3.766882	1.689484
6	0.662457	-4.105432	0.295401
6	0.594495	4.192236	0.422840
6	0.470478	3.804693	1.804535
6	0.364959	-3.343408	-2.444501
6	0.218466	-2.329929	-3.454800
6	0.207284	1.789598	3.815344
6	0.070588	0.408108	4.187460
6	-0.070596	0.417477	-4.186537
6	-0.207288	1.798133	-3.811342
6	-0.218469	-2.337658	3.449596

6	-0.364958	-3.348877	2.437035
6	-0.470472	3.808730	-1.796034
6	-0.594486	4.193177	-0.413475
6	-0.662452	-4.104762	-0.304566
6	-0.809261	-3.763088	-1.697887
6	-0.845832	3.511857	2.350743
6	-0.974175	2.523683	3.396880
6	-1.104293	-1.812131	-3.762723
6	-1.246491	-0.432681	-4.173692
6	-1.248727	-0.197343	4.211794
6	-1.390285	-1.600760	3.877042
6	-1.522714	2.327227	-3.505294
6	-1.650839	3.374925	-2.509377
6	-1.683737	-3.663092	1.927380
6	-1.829809	-4.084850	0.546435
6	-1.900284	4.214713	0.207034
6	-2.023807	3.911053	1.622844
6	-2.124124	-3.485420	-2.228393
6	-2.270441	-2.524582	-3.307324
6	-2.281323	2.016594	3.735775
6	-2.415282	0.643259	4.186141
6	-2.556726	0.169611	-4.186810
6	-2.692473	1.580011	-3.882685
6	-2.701111	-2.130393	3.598962
6	-2.847564	-3.202029	2.640206
6	-2.955806	3.686748	-1.978382
6	-3.078504	4.146581	-0.617019
6	-3.145057	-4.103439	-0.050155
6	-3.290367	-3.838667	-1.458112
6	-3.331367	3.636342	2.177570
6	-3.457923	2.709133	3.265215
6	-3.587606	-2.017369	-3.631862
6	-3.729516	-0.672822	-4.108174
6	-3.732083	0.039592	4.223018
6	-3.874866	-1.360600	3.964749
6	-4.009398	2.113609	-3.588062
6	-4.139612	3.196794	-2.662298
6	-4.171735	-3.527605	2.139875
6	-4.318305	-4.019202	0.803946
6	-4.395904	4.188775	0.003973
6	-4.526164	3.986503	1.422046
6	-4.617538	-3.581070	-2.001649
6	-4.770047	-2.705076	-3.133290
6	-4.784326	2.226840	3.639760
6	-4.917457	0.882995	4.170462
6	-5.059678	-0.074876	-4.167181
6	-5.196618	1.353320	-3.941862
6	-5.202489	-1.910276	3.735377
6	-5.350380	-3.041473	2.835839
6	-5.456892	3.551647	-2.164768
6	-5.571804	4.095668	-0.823786
6	-5.642557	-4.092130	0.215732
6	-5.779584	-3.912853	-1.218229
6	-5.840910	3.805372	2.010928
6	-5.955192	2.933978	3.208399
6	-6.092627	-2.261686	-3.533020
6	-6.224421	-0.910083	-4.127874
6	-6.220543	0.292272	4.310066
6	-6.362594	-1.159176	4.125004
6	-6.501873	1.922524	-3.728650
6	-6.633750	3.076597	-2.837274
6	-6.661852	-3.429422	2.385000
6	-6.809446	-4.005807	1.051197
6	-6.871775	4.200798	-0.204181
6	-6.976639	4.113336	1.212067
6	-7.090285	-3.707357	-1.790994
6	-7.217930	-2.934549	-2.975747
6	-7.224980	2.456478	3.699984
6	-7.352680	1.187770	4.246614
6	-7.504237	-0.256930	-4.288130

6	-7.637903	1.109856	-4.110826
6	-7.650502	-1.800034	3.948591
6	-7.792983	-2.900776	3.125207
6	-7.923613	3.523903	-2.325122
6	-8.039827	4.079888	-1.071217
6	-8.109004	-4.159088	0.404113
6	-8.245460	-4.036627	-0.958820
1	9.242114	-4.054070	1.412322
1	9.003622	-4.274770	-1.038638
1	9.030576	4.313037	0.667531
1	8.828752	3.313862	2.919220
1	8.798010	-3.286123	-2.930793
1	8.545070	-1.327487	-4.388043
1	8.640994	1.545729	4.124508
1	8.405324	-0.876469	4.432346
1	8.353603	0.822224	-4.493056
1	8.129045	3.062857	-3.521689
1	8.229701	-2.677022	3.302401
1	7.982100	4.051586	-1.638171
1	-7.982083	4.047949	1.647207
1	-8.229711	-2.669631	-3.308350
1	-8.129050	3.054963	3.528462
1	-8.353620	0.812162	4.494810
1	-8.405334	-0.866538	-4.434241
1	-8.640999	1.554966	-4.121016
1	-8.545077	-1.337313	4.385045
1	-8.798007	-3.292706	2.923452
1	-8.828745	3.320445	-2.911825
1	-9.030560	4.314596	-0.657912
1	-9.003614	-4.277143	1.029089
1	-9.242105	-4.050951	-1.421374

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B3LYP/STO-3G Energy: -6112.872520

6	-8.424821	-3.496352	-2.010387
6	-8.308894	-3.967003	-0.723913
6	-8.036003	4.379312	-0.044616
6	-7.913671	4.159253	-1.397405
6	-8.002227	-3.454119	2.231330
6	-7.847798	-2.603731	3.308846
6	-7.658322	2.271923	-3.736453
6	-7.554000	0.992996	-4.255151
6	-7.491592	0.202596	4.360665
6	-7.329144	1.564699	4.157821
6	-7.346934	-1.937895	-3.668266
6	-7.251794	-2.991511	-2.721858
6	-7.007502	3.796952	2.179734
6	-6.878716	4.241622	0.835399
6	-7.014669	-4.014443	-0.049046
6	-6.872348	-3.801588	1.387729
6	-6.626846	3.821424	-1.995489
6	-6.508792	2.930379	-3.149829
6	-6.548767	-2.058413	3.652170
6	-6.378972	-0.707005	4.202971
6	-6.291320	0.287433	-4.257729
6	-6.198696	-1.173294	-4.027923
6	-6.041371	2.121495	3.817033
6	-5.890263	3.266429	2.884163
6	-5.953128	-3.369781	-2.211901
6	-5.838653	-3.912824	-0.870740
6	-5.571735	4.264684	0.220695
6	-5.448967	4.078102	-1.213607
6	-5.558782	-3.572868	1.932646
6	-5.399276	-2.712726	3.092768
6	-5.213807	2.401031	-3.491704
6	-5.106961	1.074969	-4.074643
6	-5.061783	-0.132018	4.232103

6	-4.892556	1.299675	4.065151
6	-4.892059	-1.738508	-3.747659
6	-4.774057	-2.878425	-2.876587
6	-4.563534	3.560003	2.373596
6	-4.406906	4.113383	1.054911
6	-4.521335	-4.023971	-0.273743
6	-4.381810	-3.892363	1.144352
6	-4.133393	3.826730	-1.773661
6	-4.014803	3.013456	-2.944905
6	-4.063954	-2.271463	3.465274
6	-3.895522	-0.988843	4.075923
6	-3.792369	0.447800	-4.161652
6	-3.687906	-0.976505	-4.045617
6	-3.551089	1.829481	3.838819
6	-3.388279	2.999034	3.025795
6	-3.460220	-3.298839	-2.407208
6	-3.338778	-3.915540	-1.112828
6	-3.081402	4.195101	0.454937
6	-2.948491	4.092998	-0.976077
6	-3.057152	-3.735493	1.720831
6	-2.900944	-2.949256	2.922406
6	-2.706057	2.537856	-3.355343
6	-2.598651	1.252119	-4.011652
6	-2.565058	-0.427823	4.207177
6	-2.395556	1.010610	4.127899
6	-2.386337	-1.583899	-3.853551
6	-2.275722	-2.790450	-3.055184
6	-2.065840	3.374416	2.571851
6	-1.913503	4.022280	1.280845
6	-2.030594	-4.081053	-0.521470
6	-1.893611	-4.027392	0.922422
6	-1.642246	3.891633	-1.557735
6	-1.523807	3.131836	-2.788122
6	-1.582958	-2.540553	3.337970
6	-1.416783	-1.274616	4.025534
6	-1.302518	0.633238	-4.147135
6	-1.198035	-0.809083	-4.105306
6	-1.073721	1.556736	3.945192
6	-0.908378	2.776825	3.187676
6	-0.974546	-3.227381	-2.604394
6	-0.853524	-3.913666	-1.341092
6	-0.599508	4.124271	0.687425
6	-0.463358	4.097357	-0.747181
6	-0.575671	-3.884116	1.504881
6	-0.421339	-3.169365	2.743842
6	-0.217692	2.664960	-3.209873
6	-0.107529	1.426065	-3.931048
6	-0.085429	-0.715140	4.169790
6	0.085417	0.711284	4.170449
6	0.107526	-1.422408	-3.932367
6	0.217696	-2.661969	-3.212340
6	0.421338	3.166827	2.746776
6	0.575678	3.882725	1.508479
6	0.463368	-4.096645	-0.750977
6	0.599514	-4.124892	0.683605
6	0.853534	3.914916	-1.337464
6	0.974550	3.229805	-2.601404
6	0.908371	-2.779770	3.185109
6	1.073708	-1.560384	3.943758
6	1.198029	0.812900	-4.104564
6	1.302514	-0.629383	-4.147727
6	1.416773	1.270891	4.026717
6	1.582956	2.537462	3.340325
6	1.523814	-3.129228	-2.791018
6	1.642257	-3.890161	-1.561334
6	1.893622	4.026530	0.926155
6	2.030606	4.081531	-0.517688
6	1.913504	-4.023445	1.277123
6	2.065831	-3.376789	2.568735
6	2.275721	2.793289	-3.052605

6	2.386330	1.587482	-3.852095
6	2.395541	-1.014430	4.126978
6	2.565045	0.423926	4.207587
6	2.598649	-1.248382	-4.012818
6	2.706064	-2.534722	-3.357690
6	2.900949	2.946536	2.925138
6	3.057166	3.733878	1.724289
6	2.948502	-4.092053	-0.979859
6	3.081406	-4.195491	0.451060
6	3.338789	3.916556	-1.109200
6	3.460223	3.301069	-2.404159
6	3.388265	-3.001834	3.023040
6	3.551072	-1.833042	3.837154
6	3.687897	0.980270	-4.044741
6	3.792365	-0.443925	-4.162088
6	3.895515	0.985058	4.076857
6	4.063957	2.268235	3.467386
6	4.014815	-3.010686	-2.947684
6	4.133407	-3.825036	-1.777187
6	4.381828	3.891266	1.147954
6	4.521351	4.024191	-0.270020
6	4.406903	-4.114338	1.051120
6	4.563520	-3.562207	2.370333
6	4.774056	2.881101	-2.873946
6	4.892049	1.742003	-3.746097
6	4.892539	-1.303458	4.063992
6	5.061770	0.128081	4.232262
6	5.106960	-1.071167	-4.075664
6	5.213817	-2.397756	-3.493922
6	5.399284	2.709824	3.095283
6	5.558800	3.571024	1.935947
6	5.448979	-4.076915	-1.217358
6	5.571734	-4.264855	0.216769
6	5.838665	3.913590	-0.867126
6	5.953129	3.371825	-2.208805
6	5.890245	-3.269135	2.881201
6	6.041352	-2.125065	3.815140
6	6.198683	1.177063	-4.026924
6	6.291315	-0.283457	-4.258070
6	6.378962	0.703084	4.203670
6	6.548770	2.054985	3.654087
6	6.508805	-2.927408	-3.152527
6	6.626866	-3.819503	-1.998992
6	6.872369	3.800222	1.391233
6	7.014688	4.014409	-0.045344
6	6.878707	-4.242396	0.831513
6	7.007475	-3.799051	2.176298
6	7.251791	2.994048	-2.719144
6	7.346917	1.941367	-3.666605
6	7.329123	-1.568596	4.156492
6	7.491575	-0.206675	4.360573
6	7.553997	-0.989031	-4.256175
6	7.658329	-2.268424	-3.738596
6	7.847806	2.600597	3.311255
6	8.002245	3.451954	2.234510
6	7.913683	-4.157899	-1.401204
6	8.036000	-4.379256	-0.048626
6	8.308910	3.967589	-0.720267
6	8.424826	3.498189	-2.007190
1	-9.415451	-3.369128	-2.468954
1	-9.213833	-4.221531	-0.157095
1	-9.027037	4.529473	0.406168
1	-8.814055	4.139125	-2.025075
1	-9.012305	-3.760220	1.929849
1	-8.738050	-2.248630	3.844083
1	-8.650607	2.731248	-3.640580
1	-8.466768	0.464328	-4.559536
1	-8.503905	-0.199867	4.495465
1	-8.217549	2.209375	4.137339
1	-8.348665	-1.570996	-3.928514

1	-8.021170	3.648655	2.575052
1	8.021085	-3.651211	2.571776
1	8.348594	1.574787	-3.927275
1	8.217516	-2.213263	4.135482
1	8.503877	0.195659	4.495783
1	8.466751	-0.460108	-4.560137
1	8.650596	-2.727840	-3.643163
1	8.738058	2.244999	3.846167
1	9.012336	3.758312	1.933300
1	8.814078	-4.137195	-2.028844
1	9.027024	-4.529877	0.402015
1	9.213862	4.221555	-0.153209
1	9.415463	3.371398	-2.465881

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B3LYP/STO-3G Energy: -6188.167752

6	-8.502888	-3.007838	-2.749318
6	-8.354518	-3.788767	-1.628181
6	-8.219085	4.103244	1.158160
6	-8.116172	4.239459	-0.206785
6	-8.000544	-4.045181	1.354550
6	-7.841079	-3.496611	2.611537
6	-7.867775	3.022478	-2.955047
6	-7.750238	1.922490	-3.785639
6	-7.517937	-1.046384	4.341887
6	-7.385205	0.324974	4.492636
6	-7.482419	-1.056101	-3.969461
6	-7.351877	-2.312552	-3.324667
6	-7.140971	2.995856	3.147034
6	-7.043919	3.770472	1.959981
6	-7.046369	-3.979423	-1.005823
6	-6.880307	-4.138583	0.433829
6	-6.833251	4.094037	-0.887195
6	-6.719292	3.532339	-2.231697
6	-6.545262	-3.027368	3.065100
6	-6.390739	-1.859918	3.941086
6	-6.474905	1.267262	-3.983824
6	-6.353117	-0.200131	-4.137397
6	-6.113897	0.980218	4.288941
6	-6.000987	2.327848	3.679348
6	-6.037075	-2.781877	-2.947217
6	-5.887870	-3.646913	-1.791488
6	-5.747991	3.979881	1.355894
6	-5.646597	4.168725	-0.079687
6	-5.560459	-4.028482	1.001283
6	-5.394475	-3.490771	2.341013
6	-5.421139	3.136677	-2.714283
6	-5.301448	2.006987	-3.619927
6	-5.084194	-1.281754	4.100310
6	-4.945362	0.148614	4.304909
6	-5.032850	-0.790542	-4.029730
6	-4.879685	-2.113036	-3.481279
6	-4.689682	2.773044	3.245728
6	-4.566638	3.647896	2.109879
6	-4.558290	-3.878769	-1.261381
6	-4.393759	-4.109514	0.141463
6	-4.337043	4.097274	-0.701256
6	-4.224233	3.612991	-2.042799
6	-4.061211	-3.128355	2.795156
6	-3.905540	-2.042046	3.712604
6	-3.978336	1.450830	-3.880599
6	-3.847467	0.047967	-4.136650
6	-3.619092	0.749266	4.205546
6	-3.493019	2.090874	3.718390
6	-3.550573	-2.611614	-3.153252
6	-3.394086	-3.534283	-2.061865
6	-3.253562	3.908844	1.534272

6	-3.143219	4.176303	0.124049
6	-3.060812	-4.073296	0.720253
6	-2.895887	-3.616062	2.078876
6	-2.913786	3.285290	-2.576614
6	-2.795300	2.214768	-3.542233
6	-2.583169	-1.502374	3.965430
6	-2.442419	-0.090484	4.258975
6	-2.531959	-0.560995	-4.125111
6	-2.386416	-1.929369	-3.667046
6	-2.185539	2.600636	3.360225
6	-2.067882	3.558371	2.276100
6	-2.071436	-3.817681	-1.551073
6	-1.907093	-4.127624	-0.143306
6	-1.843030	4.158225	-0.505430
6	-1.732299	3.739480	-1.890287
6	-1.577118	-3.296196	2.566493
6	-1.421898	-2.246813	3.555085
6	-1.491501	1.679377	-3.849245
6	-1.361918	0.277410	-4.184075
6	-1.134571	0.515028	4.209279
6	-1.006344	1.893038	3.790400
6	-1.070833	-2.440974	-3.363763
6	-0.914130	-3.424968	-2.319323
6	-0.766775	3.837995	1.713071
6	-0.655012	4.177533	0.316292
6	-0.581272	-4.106273	0.436807
6	-0.416180	-3.724008	1.814666
6	-0.426066	3.422895	-2.432506
6	-0.306880	2.413498	-3.449190
6	-0.100001	-1.712648	3.821423
6	0.043934	-0.332078	4.192740
6	-0.043933	-0.332297	-4.192724
6	0.100002	-1.712849	-3.821335
6	0.306880	2.413680	3.449065
6	0.426065	3.423024	2.432328
6	0.416180	-3.724105	-1.814473
6	0.581272	-4.106297	-0.436595
6	0.655011	4.177517	-0.316509
6	0.766774	3.837905	-1.713271
6	0.914130	-3.424845	2.319499
6	1.070834	-2.440797	3.363888
6	1.006344	1.892839	-3.790497
6	1.134572	0.514807	-4.209305
6	1.361919	0.277629	4.184060
6	1.491501	1.679580	3.849158
6	1.421899	-2.247001	-3.554969
6	1.577118	-3.296332	-2.566323
6	1.732298	3.739582	1.890092
6	1.843029	4.158254	0.505214
6	1.907092	-4.127617	0.143520
6	2.071436	-3.817600	1.551271
6	2.067881	3.558252	-2.276284
6	2.185539	2.600459	-3.360358
6	2.386416	-1.929176	3.667143
6	2.531960	-0.560778	4.125137
6	2.442420	-0.090707	-4.258968
6	2.583170	-1.502582	-3.965351
6	2.795300	2.214955	3.542117
6	2.913785	3.285428	2.576443
6	2.895886	-3.616174	-2.078689
6	3.060811	-4.073336	-0.720042
6	3.143218	4.176300	-0.124267
6	3.253562	3.908765	-1.534475
6	3.394086	-3.534175	2.062047
6	3.550573	-2.611448	3.153385
6	3.493020	2.090678	-3.718495
6	3.619093	0.749045	-4.205581
6	3.847468	0.048185	4.136644
6	3.978336	1.451034	3.880521
6	3.905540	-2.042241	-3.712497

6	4.061211	-3.128504	-2.794994
6	4.224232	3.613102	2.042610
6	4.337041	4.097316	0.701043
6	4.393759	-4.109525	-0.141250
6	4.558289	-3.878705	1.261582
6	4.566638	3.647787	-2.110067
6	4.689682	2.772874	-3.245868
6	4.879686	-2.112853	3.481385
6	5.032851	-0.790330	4.029766
6	4.945363	0.148388	-4.304912
6	5.084195	-1.281969	-4.100240
6	5.301448	2.007178	3.619819
6	5.421138	3.136822	2.714118
6	5.394475	-3.490898	-2.340832
6	5.560458	-4.028540	-1.001074
6	5.646595	4.168735	0.079470
6	5.747991	3.979813	-1.356100
6	5.887870	-3.646821	1.791677
6	6.037075	-2.781722	2.947358
6	6.000988	2.327652	-3.679460
6	6.113898	0.979991	-4.288982
6	6.353117	-0.199913	4.137399
6	6.474905	1.267472	3.983751
6	6.390740	-1.860124	-3.940984
6	6.545262	-3.027530	-3.064942
6	6.719291	3.532460	2.231512
6	6.833249	4.094090	0.886983
6	6.880306	-4.138611	-0.433615
6	7.046368	-3.979375	1.006029
6	7.043920	3.770368	-1.960173
6	7.140974	2.995682	-3.147179
6	7.351878	-2.312376	3.324781
6	7.482421	-1.055891	3.969504
6	7.385207	0.324739	-4.492636
6	7.517939	-1.046610	-4.341820
6	7.750238	1.922688	3.785529
6	7.867775	3.022635	2.954884
6	7.841079	-3.496751	-2.611354
6	8.000543	-4.045259	-1.354341
6	8.116170	4.239478	0.206566
6	8.219085	4.103188	-1.158371
6	8.354517	-3.788685	1.628376
6	8.502888	-3.007694	2.749470
1	-9.503673	-2.789347	-3.146853
1	-9.243606	-4.199678	-1.132648
1	-9.204349	4.111479	1.644495
1	-9.026235	4.361486	-0.808270
1	-9.009944	-4.287769	0.998716
1	-8.726542	-3.311862	3.233393
1	-8.865373	3.423081	-2.734351
1	-8.657980	1.471478	-4.207044
1	-8.519050	-1.494156	4.384330
1	-8.285277	0.932970	4.651311
1	-8.494053	-0.655871	-4.114997
1	-8.143835	2.729039	3.504397
1	8.143835	2.728838	-3.504519
1	8.494057	-0.655648	4.115013
1	8.285279	0.932729	-4.651334
1	8.519054	-1.494383	-4.384235
1	8.657981	1.471696	4.206955
1	8.865372	3.423226	2.734167
1	8.726542	-3.312034	-3.233219
1	9.009943	-4.287830	-0.998495
1	9.026233	4.361539	0.808046
1	9.204347	4.111401	-1.644706
1	9.243605	-4.199624	1.132865
1	9.503673	-2.789181	3.146992

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B3LYP/STO-3G Energy: -6263.462678

6	-8.581341	-2.089801	-3.547894
6	-8.466972	-3.133832	-2.661945
6	-8.302706	3.772283	2.052083
6	-8.167592	4.252324	0.770551
6	-8.179695	-4.153053	0.161205
6	-8.040135	-3.948057	1.518956
6	-7.869708	3.779214	-2.193285
6	-7.745775	2.927422	-3.275418
6	-7.725527	-2.029899	3.825817
6	-7.581095	-0.745824	4.324965
6	-7.510108	0.090671	-4.208818
6	-7.409347	-1.290136	-3.905184
6	-7.280344	2.175383	3.710169
6	-7.149042	3.225890	2.764259
6	-7.174652	-3.500401	-2.085905
6	-7.041115	-4.025624	-0.733606
6	-6.870707	4.265498	0.099847
6	-6.732037	4.065871	-1.340098
6	-6.748164	-3.631684	2.100176
6	-6.598622	-2.731260	3.248051
6	-6.473504	2.321696	-3.609550
6	-6.366082	0.941697	-4.131223
6	-6.298017	-0.080093	4.317449
6	-6.158113	1.375792	4.075931
6	-6.108579	-1.864048	-3.637945
6	-5.995179	-2.998709	-2.740731
6	-5.837340	3.564073	2.259485
6	-5.701598	4.112818	0.922691
6	-5.731993	-4.088047	-0.133938
6	-5.587682	-3.913971	1.301548
6	-5.427321	3.785602	-1.883298
6	-5.299793	2.923442	-3.045862
6	-5.289209	-2.234439	3.573199
6	-5.139151	-0.906494	4.140658
6	-5.056029	0.320367	-4.154913
6	-4.931613	-1.101484	-3.962322
6	-4.833707	1.897381	3.796669
6	-4.676868	3.032622	2.925937
6	-4.680647	-3.382693	-2.265302
6	-4.548830	-3.967108	-0.965349
6	-4.379670	4.182186	0.328838
6	-4.241278	4.054060	-1.089483
6	-4.260497	-3.701109	1.856099
6	-4.111534	-2.887963	3.023096
6	-3.978175	2.428872	-3.413848
6	-3.858507	1.136938	-4.019151
6	-3.805005	-0.321293	4.221280
6	-3.654531	1.097535	4.098970
6	-3.616646	-1.691057	-3.749862
6	-3.495414	-2.865117	-2.930443
6	-3.348821	3.412176	2.461527
6	-3.204000	4.028732	1.170119
6	-3.227912	-4.102172	-0.373242
6	-3.085716	-4.008534	1.058454
6	-2.922175	3.849699	-1.663459
6	-2.793589	3.059207	-2.866297
6	-2.787916	-2.451271	3.427600
6	-2.637786	-1.165470	4.076352
6	-2.550585	0.521945	-4.139398
6	-2.432272	-0.919439	-4.049274
6	-2.333698	1.662327	3.908980
6	-2.182612	2.865257	3.112177
6	-2.187170	-3.294239	-2.486880
6	-2.056493	-3.955574	-1.203023
6	-1.889447	4.152374	0.582035
6	-1.751025	4.096063	-0.860891
6	-1.773145	-3.845215	1.634190

6	-1.626492	-3.084631	2.860274
6	-1.488761	2.596893	-3.274294
6	-1.368607	1.326308	-3.956971
6	-1.322949	-0.588413	4.207892
6	-1.171536	0.849469	4.163150
6	-1.130136	-1.516259	-3.866931
6	-1.008912	-2.739700	-3.109659
6	-0.867518	3.261874	2.666405
6	-0.720894	3.946189	1.405000
6	-0.743396	-4.106048	-0.614129
6	-0.602546	-4.087365	0.818686
6	-0.436700	3.904843	-1.439181
6	-0.305621	3.182492	-2.676026
6	-0.304898	-2.656593	3.276015
6	-0.153543	-1.420299	3.992053
6	-0.059305	0.716040	-4.097924
6	0.059304	-0.716074	-4.097918
6	0.153543	1.420331	3.992041
6	0.304898	2.656619	3.275993
6	0.305621	-3.182514	-2.676000
6	0.436699	-3.904855	-1.439149
6	0.602546	4.087372	0.818653
6	0.743395	4.106043	-0.614162
6	0.720894	-3.946178	1.405032
6	0.867518	-3.261853	2.666431
6	1.008912	2.739675	-3.109682
6	1.130136	1.516227	-3.866943
6	1.171537	-0.849435	4.163157
6	1.322949	0.588447	4.207887
6	1.368607	-1.326341	-3.956960
6	1.488761	-2.596919	-3.274273
6	1.626492	3.084654	2.860249
6	1.773145	3.845228	1.634159
6	1.751025	-4.096071	-0.860858
6	1.889447	-4.152370	0.582069
6	2.056493	3.955564	-1.203055
6	2.187170	3.294219	-2.486908
6	2.182613	-2.865232	3.112200
6	2.333699	-1.662295	3.908994
6	2.432272	0.919406	-4.049282
6	2.550585	-0.521979	-4.139394
6	2.637787	1.165503	4.076343
6	2.787916	2.451300	3.427580
6	2.793589	-3.059231	-2.866273
6	2.922174	-3.849714	-1.663428
6	3.085716	4.008542	1.058421
6	3.227912	4.102169	-0.373276
6	3.204000	-4.028723	1.170152
6	3.348821	-3.412156	2.461555
6	3.495414	2.865093	-2.930467
6	3.616646	1.691026	-3.749876
6	3.654531	-1.097501	4.098978
6	3.805005	0.321328	4.221277
6	3.858507	-1.136970	-4.019142
6	3.978175	-2.428901	-3.413829
6	4.111533	2.887988	3.023072
6	4.260496	3.701124	1.856069
6	4.241277	-4.054070	-1.089450
6	4.379670	-4.182183	0.328872
6	4.548830	3.967099	-0.965382
6	4.680646	3.382674	-2.265330
6	4.676868	-3.032597	2.925960
6	4.833708	-1.897349	3.796682
6	4.931613	1.101452	-3.962331
6	5.056029	-0.320401	-4.154909
6	5.139152	0.906528	4.140650
6	5.289209	2.234468	3.573180
6	5.299792	-2.923467	-3.045838
6	5.427320	-3.785618	-1.883268
6	5.587682	3.913981	1.301516

6	5.731993	4.088046	-0.133971
6	5.701598	-4.112811	0.922724
6	5.837341	-3.564055	2.259512
6	5.995179	2.998687	-2.740755
6	6.108579	1.864018	-3.637959
6	6.158114	-1.375758	4.075940
6	6.298018	0.080129	4.317448
6	6.366082	-0.941731	-4.131214
6	6.473504	-2.321726	-3.609530
6	6.598622	2.731287	3.248029
6	6.748164	3.631702	2.100146
6	6.732036	-4.065884	-1.340067
6	6.870706	-4.265500	0.099881
6	7.041115	4.025619	-0.733639
6	7.174652	3.500385	-2.085934
6	7.149043	-3.225867	2.764284
6	7.280345	-2.175351	3.710183
6	7.409347	1.290104	-3.905193
6	7.510109	-0.090706	-4.208812
6	7.581095	0.745860	4.324960
6	7.725526	2.029932	3.825801
6	7.745774	-2.927448	-3.275394
6	7.869707	-3.779232	-2.193254
6	8.040134	3.948071	1.518923
6	8.179694	4.153055	0.161171
6	8.167592	-4.252319	0.770585
6	8.302706	-3.772267	2.052112
6	8.466972	3.133810	-2.661970
6	8.581341	2.089771	-3.547909
1	-9.570458	-1.759542	-3.894450
1	-9.371480	-3.642702	-2.304413
1	-9.298485	3.671785	2.505824
1	-9.062285	4.539969	0.203384
1	-9.184033	-4.280441	-0.262554
1	-8.935900	-3.915443	2.152547
1	-8.867057	4.128835	-1.897450
1	-8.648207	2.616636	-3.817665
1	-8.731784	-2.458902	3.736308
1	-8.477071	-0.184749	4.620628
1	-8.512939	0.532800	-4.266130
1	-8.293328	1.841151	3.968643
1	8.293331	-1.841115	3.968651
1	8.512939	-0.532836	-4.266124
1	8.477071	0.184787	4.620626
1	8.731782	2.458933	3.736286
1	8.648207	-2.616664	-3.817640
1	8.867056	-4.128848	-1.897415
1	8.935899	3.915462	2.152514
1	9.184032	4.280441	-0.262589
1	9.062284	-4.539969	0.203420
1	9.298484	-3.671765	2.505852
1	9.371480	3.642682	-2.304440
1	9.570459	1.759508	-3.894459

Nanotube (7,5) u07v00
B3LYP/STO-3G Energy: -6338.757242

6	8.752373	-1.186095	3.830570
6	8.613131	-2.420270	3.243973
6	8.383098	3.045242	-3.081930
6	8.280362	3.838621	-1.963863
6	8.257736	-4.123537	0.780470
6	8.088191	-4.271527	-0.580740
6	8.045589	4.144660	1.028123
6	7.939863	3.600899	2.294428
6	7.729412	-3.008331	-3.296847
6	7.580302	-1.894559	-4.105757
6	7.707726	1.102304	3.929273

6	7.592507	-0.307857	3.992435
6	7.312303	1.089361	-4.253341
6	7.209669	2.347992	-3.606551
6	7.306072	-2.907748	2.805629
6	7.139886	-3.759205	1.636811
6	6.998709	4.038835	-1.292521
6	6.890798	4.216273	0.151867
6	6.784068	-4.101116	-1.196885
6	6.612240	-3.524370	-2.532944
6	6.670764	3.115598	2.797680
6	6.566193	1.918062	3.657699
6	6.301027	-1.233569	-4.241038
6	6.175865	0.235967	-4.378517
6	6.282546	-0.917045	3.907534
6	6.143557	-2.242646	3.334591
6	5.911670	2.821071	-3.179492
6	5.810007	3.695835	-2.026107
6	5.816921	-3.960907	1.100620
6	5.640666	-4.158729	-0.328300
6	5.596343	4.101321	0.774764
6	5.488677	3.567159	2.121879
6	5.297884	-3.113293	-2.947260
6	5.141719	-1.973556	-3.833408
6	5.253729	1.338358	3.866007
6	5.117248	-0.084141	4.047981
6	4.861871	0.827858	-4.215831
6	4.732811	2.151119	-3.663682
6	4.817458	-2.722137	3.000903
6	4.653963	-3.619483	1.897655
6	4.502749	3.932216	-1.443967
6	4.395209	4.172591	-0.037504
6	4.302661	-4.080983	-0.890893
6	4.130407	-3.590683	-2.223191
6	4.172788	3.197791	2.629510
6	4.058238	2.105514	3.547100
6	3.809910	-1.412465	-4.031688
6	3.671024	-0.008667	-4.275564
6	3.794728	-0.694077	4.019119
6	3.649514	-2.037523	3.533428
6	3.418610	2.653734	-3.285560
6	3.307376	3.582842	-2.194407
6	3.319254	-3.888475	1.387266
6	3.144900	-4.162207	-0.016113
6	3.087581	4.137123	0.595695
6	2.979791	3.680966	1.961300
6	2.799303	-3.255557	-2.696743
6	2.640797	-2.177184	-3.647757
6	2.748801	1.556004	3.845638
6	2.620339	0.142056	4.131932
6	2.357981	0.602229	-4.209060
6	2.233298	1.971256	-3.749195
6	2.329141	-2.553464	3.242659
6	2.166868	-3.522768	2.176830
6	2.006825	3.870815	-1.631905
6	1.900142	4.186416	-0.220655
6	1.819588	-4.138873	-0.586957
6	1.647597	-3.712252	-1.962149
6	1.680956	3.353303	2.499191
6	1.567782	2.299907	3.485855
6	1.325961	-1.637314	-3.893843
6	1.184450	-0.234621	-4.218846
6	1.311645	-0.467448	4.135432
6	1.167805	-1.844598	3.723979
6	0.931543	2.487312	-3.396050
6	0.818757	3.476664	-2.351646
6	0.841239	-3.808271	1.674790
6	0.667825	-4.155985	0.287737
6	0.598225	4.165467	0.412887
6	0.489411	3.781218	1.794888
6	0.319313	-3.388565	-2.443197

6	0.157757	-2.371336	-3.445595
6	0.258481	1.760057	3.802157
6	0.131647	0.377848	4.172803
6	-0.131660	0.377351	-4.172846
6	-0.258490	1.759603	-3.802359
6	-0.157762	-2.370924	3.445870
6	-0.319310	-3.388273	2.443593
6	-0.489402	3.781004	-1.795330
6	-0.598212	4.165423	-0.413376
6	-0.667813	-4.156027	-0.287248
6	-0.841231	-3.808480	-1.674342
6	-0.818753	3.476954	2.351238
6	-0.931548	2.487722	3.395755
6	-1.167813	-1.845044	-3.723756
6	-1.311658	-0.467941	-4.135363
6	-1.184465	-0.234118	4.218858
6	-1.325972	-1.636850	3.894020
6	-1.567787	2.299492	-3.486111
6	-1.680952	3.353010	-2.499578
6	-1.647590	-3.712030	1.962582
6	-1.819576	-4.138823	0.587443
6	-1.900129	4.186465	0.220163
6	-2.006817	3.871031	1.631449
6	-2.166863	-3.523045	-2.176414
6	-2.329144	-2.553859	-3.242350
6	-2.233306	1.971706	3.748945
6	-2.357996	0.602730	4.208960
6	-2.620350	0.141562	-4.131919
6	-2.748809	1.555545	-3.845794
6	-2.640806	-2.176752	3.647991
6	-2.799302	-3.255249	2.697115
6	-2.979783	3.680752	-1.961729
6	-3.087568	4.137085	-0.596183
6	-3.144887	-4.162241	0.016602
6	-3.319244	-3.888673	-1.386809
6	-3.307372	3.583129	2.193979
6	-3.418615	2.654136	3.285228
6	-3.649520	-2.037951	-3.533165
6	-3.794738	-0.694558	-4.018999
6	-3.671039	-0.008158	4.275519
6	-3.809924	-1.411986	4.031814
6	-4.058243	2.105095	-3.547317
6	-4.172783	3.197496	-2.629873
6	-4.130403	-3.590447	2.223604
6	-4.302649	-4.080922	0.891371
6	-4.395197	4.172645	0.037009
6	-4.502741	3.932432	1.443499
6	-4.653956	-3.619746	-1.897226
6	-4.817459	-2.722513	-3.000565
6	-4.732819	2.151563	3.663393
6	-4.861885	0.828360	4.215680
6	-5.117258	-0.084624	-4.047917
6	-5.253736	1.337899	-3.866116
6	-5.141732	-1.973103	3.833596
6	-5.297886	-3.112964	2.947605
6	-5.488669	3.566942	-2.122294
6	-5.596331	4.101287	-0.775251
6	-5.640653	-4.158755	0.328787
6	-5.816910	-3.961097	-1.100156
6	-5.810001	3.696121	2.025660
6	-5.911673	2.821472	3.179131
6	-6.143561	-2.243056	-3.334291
6	-6.282555	-0.917512	-3.907366
6	-6.175881	0.236492	4.378432
6	-6.301046	-1.233064	4.241122
6	-6.566197	1.917633	-3.657877
6	-6.670760	3.115295	-2.798030
6	-6.612238	-3.524112	2.533342
6	-6.784056	-4.101047	1.197363
6	-6.890785	4.216332	-0.152371

6	-6.998700	4.039056	1.292036
6	-7.139877	-3.759462	-1.636366
6	-7.306072	-2.908111	-2.805260
6	-7.209674	2.348446	3.606242
6	-7.312310	1.089890	4.253181
6	-7.592515	-0.308332	-3.992322
6	-7.707732	1.101839	-3.929333
6	-7.580317	-1.894082	4.105920
6	-7.729415	-3.007971	3.297166
6	-7.939855	3.600686	-2.294850
6	-8.045576	4.144624	-1.028621
6	-8.088177	-4.271564	0.581238
6	-8.257723	-4.123726	-0.779988
6	-8.280355	3.838919	1.963397
6	-8.383098	3.045653	3.081545
6	-8.613134	-2.420671	-3.243635
6	-8.752381	-1.186551	-3.830347
1	9.750324	-0.789314	4.063333
1	9.506531	-3.014528	3.012372
1	9.367406	2.820337	-3.515571
1	9.189402	4.251565	-1.507755
1	9.270709	-4.149368	1.202143
1	8.969111	-4.412533	-1.220269
1	9.038249	4.396059	0.633099
1	8.851566	3.430220	2.881508
1	8.734778	-3.412997	-3.123021
1	8.471560	-1.439441	-4.556902
1	8.713781	1.533806	3.852242
1	8.316548	0.687347	-4.438538
1	-8.316552	0.687916	4.438459
1	-8.713785	1.533350	-3.852357
1	-8.471582	-1.438911	4.556999
1	-8.734776	-3.412668	3.123392
1	-8.851559	3.429939	-2.881909
1	-9.038235	4.396090	-0.633632
1	-8.969093	-4.412519	1.220782
1	-9.270696	-4.149621	-1.201664
1	-9.189392	4.251827	1.507246
1	-9.367407	2.820806	3.515209
1	-9.506533	-3.014905	-3.011966
1	-9.750335	-0.789791	-4.063137

Nanotube (7,5) u07v01
B3LYP/STO-3G Energy: -6414.051584

6	8.762932	0.128029	-4.162993
6	8.637171	1.471839	-3.909395
6	8.558792	-2.186000	3.614806
6	8.431786	-3.238452	2.740141
6	8.340626	3.750358	-1.955622
6	8.203313	4.242688	-0.674495
6	8.129102	-4.299375	-0.068273
6	7.993044	-4.098123	-1.428385
6	7.907165	3.721380	2.282875
6	7.776354	2.853932	3.353415
6	7.718201	-2.102962	-3.645489
6	7.600014	-0.756345	-4.065269
6	7.512592	0.009792	4.268405
6	7.396401	-1.370933	3.968272
6	7.340673	2.062598	-3.578991
6	7.202457	3.185413	-2.664595
6	7.135052	-3.597747	2.170428
6	6.994502	-4.138691	0.823784
6	6.913558	4.244096	-0.005607
6	6.772458	4.030507	1.436220
6	6.711036	-3.752346	-2.010371
6	6.583965	-2.815856	-3.145428
6	6.499859	2.256576	3.681661

6	6.377943	0.873335	4.194318
6	6.291550	-0.138423	-4.108264
6	6.165626	1.290255	-3.892330
6	6.089082	-1.931639	3.705772
6	5.962460	-3.072960	2.818735
6	5.892311	3.526791	-2.168368
6	5.749908	4.085663	-0.834524
6	5.685577	-4.183275	0.221832
6	5.545707	-4.011800	-1.214543
6	5.467707	3.748255	1.971711
6	5.331488	2.874445	3.123722
6	5.266240	-2.302377	-3.464784
6	5.123845	-0.973100	-4.002379
6	5.061373	0.266362	4.217636
6	4.920976	-1.154017	4.027059
6	4.847996	1.847015	-3.662568
6	4.710971	2.999494	-2.824213
6	4.643215	-3.445482	2.346795
6	4.504138	-4.039106	1.052234
6	4.425889	4.163938	-0.240993
6	4.284399	4.031825	1.175905
6	4.218290	-3.778689	-1.769296
6	4.080012	-2.956059	-2.931849
6	4.004988	2.389617	3.487360
6	3.871697	1.096311	4.084925
6	3.802080	-0.368985	-4.098413
6	3.667813	1.054503	-3.971886
6	3.599004	-1.730111	3.818865
6	3.464309	-2.908082	3.008011
6	3.388959	3.399045	-2.369765
6	3.247938	4.025529	-1.081463
6	3.182066	-4.161967	0.460813
6	3.041793	-4.070194	-0.971807
6	2.964173	3.836523	1.748842
6	2.826714	3.037724	2.945434
6	2.762437	-2.493640	-3.329091
6	2.625272	-1.200059	-3.963113
6	2.556934	0.495505	4.205007
6	2.422766	-0.944489	4.116248
6	2.354095	1.635772	-3.792588
6	2.217401	2.848644	-3.011997
6	2.151247	-3.326510	2.568571
6	2.013128	-3.996174	1.290074
6	1.935990	4.159350	-0.494133
6	1.795673	4.099485	0.947473
6	1.729790	-3.886543	-1.546076
6	1.590988	-3.117215	-2.764636
6	1.517601	2.586109	3.349894
6	1.383568	1.313136	4.025217
6	1.315812	-0.604769	-4.090831
6	1.181210	0.833129	-4.045817
6	1.114268	-1.527696	3.936895
6	0.979404	-2.754152	3.187565
6	0.904383	3.264314	-2.571901
6	0.764358	3.960485	-1.318075
6	0.698219	-4.135759	0.702631
6	0.556760	-4.118351	-0.729381
6	0.479332	3.917764	1.524408
6	0.340199	3.188485	2.755183
6	0.274164	-2.668973	-3.175190
6	0.136544	-1.424417	-3.880522
6	0.067209	0.716598	4.164209
6	-0.067220	-0.713295	4.164772
6	-0.136549	1.421339	-3.881642
6	-0.274164	2.666451	-3.177293
6	-0.340199	-3.186296	2.757698
6	-0.479327	-3.916553	1.527503
6	-0.556751	4.117773	-0.732636
6	-0.698212	4.136321	0.699362
6	-0.764350	-3.961537	-1.314946

6	-0.904380	-3.266359	-2.569322
6	-0.979406	2.756684	3.185388
6	-1.114277	1.530820	3.935683
6	-1.181216	-0.836337	-4.045152
6	-1.315819	0.601524	-4.091298
6	-1.383578	-1.309943	4.026241
6	-1.517606	-2.583451	3.351926
6	-1.590986	3.115022	-2.767092
6	-1.729783	3.885321	-1.549146
6	-1.795666	-4.098742	0.950711
6	-1.935981	-4.159755	-0.490847
6	-2.013121	3.997212	1.286915
6	-2.151245	3.328559	2.565940
6	-2.217399	-2.851041	-3.009744
6	-2.354099	-1.638782	-3.791287
6	-2.422776	0.947754	4.115485
6	-2.556945	-0.492170	4.205375
6	-2.625278	1.196914	-3.964041
6	-2.762438	2.490999	-3.331046
6	-2.826717	-3.035390	2.947821
6	-2.964168	-3.835147	1.751869
6	-3.041785	4.069439	-0.975023
6	-3.182057	4.162355	0.457523
6	-3.247929	-4.026410	-1.078284
6	-3.388954	-3.400942	-2.367079
6	-3.464310	2.910481	3.005706
6	-3.599011	1.733144	3.817480
6	-3.667818	-1.057655	-3.971033
6	-3.802087	0.365734	-4.098677
6	-3.871708	-1.093070	4.085758
6	-4.004994	-2.386851	3.489223
6	-4.080012	2.953737	-2.934170
6	-4.218284	3.777301	-1.772277
6	-4.284392	-4.030916	1.179086
6	-4.425879	-4.164161	-0.237706
6	-4.504130	4.039973	1.049041
6	-4.643212	3.447368	2.344068
6	-4.710968	-3.001753	-2.821839
6	-4.847999	-1.849927	-3.661090
6	-4.920985	1.157215	4.026116
6	-5.061385	-0.263015	4.217805
6	-5.123852	0.969924	-4.003111
6	-5.266243	2.299629	-3.466575
6	-5.331492	-2.871972	3.125967
6	-5.467704	-3.746712	1.974661
6	-5.545700	4.010866	-1.217712
6	-5.685567	4.183493	0.218525
6	-5.749898	-4.086368	-0.831300
6	-5.892303	-3.528544	-2.165583
6	-5.962459	3.075221	2.816297
6	-6.089088	1.934588	3.704219
6	-6.165631	-1.293348	-3.891278
6	-6.291558	0.135161	-4.108328
6	-6.377955	-0.870005	4.194957
6	-6.499868	-2.253655	3.683402
6	-6.583965	2.813367	-3.147627
6	-6.711030	3.750778	-2.013328
6	-6.772453	-4.029404	1.439394
6	-6.913547	-4.244154	-0.002261
6	-6.994493	4.139398	0.820512
6	-7.135047	3.599510	2.167579
6	-7.202452	-3.187561	-2.662074
6	-7.340675	-2.065450	-3.577334
6	-7.396409	1.374090	3.967147
6	-7.512603	-0.006402	4.268356
6	-7.600022	0.753116	-4.065809
6	-7.718205	2.100070	-3.647103
6	-7.776360	-2.851278	3.355628
6	-7.907163	-3.719595	2.285793
6	-7.993035	4.097039	-1.431622

6	-8.129091	4.299387	-0.071673
6	-8.203302	-4.243292	-0.671153
6	-8.340616	-3.751968	-1.952665
6	-8.431784	3.240662	2.737567
6	-8.558797	2.188885	3.613042
6	-8.637176	-1.474948	-3.908180
6	-8.762940	-0.131334	-4.162820
1	9.755045	-0.320655	-4.310995
1	9.535265	2.101126	-3.860420
1	9.552239	-1.862738	3.955612
1	9.330447	-3.759943	2.385966
1	9.343208	3.661445	-2.393179
1	9.098910	4.537740	-0.112573
1	9.130800	-4.446275	0.355458
1	8.890254	-4.088776	-2.060785
1	8.908023	4.063100	1.989392
1	8.677232	2.525738	3.887924
1	8.726327	-2.506387	-3.485344
1	8.520475	0.441009	4.323880
1	-8.520493	-0.437576	4.324157
1	-8.726334	2.503621	-3.487272
1	-8.677243	-2.522652	3.889865
1	-8.908019	-4.061556	1.992583
1	-8.890246	4.087194	-2.064015
1	-9.130786	4.446640	0.351939
1	-9.098896	-4.537916	-0.109001
1	-9.343197	-3.663411	-2.390296
1	-9.330442	3.761884	2.382986
1	-9.552247	1.865888	3.954094
1	-9.535269	-2.104195	-3.858705
1	-9.755058	0.317234	-4.311154

Nanotube (7,5) u07v02
B3LYP/STO-3G Energy: -6489.345682

6	8.953275	3.909655	-0.944575
6	8.830082	4.010809	0.419132
6	8.571138	-4.199275	-1.195236
6	8.456577	-3.620039	-2.435988
6	8.508280	2.711374	3.121960
6	8.348535	1.602028	3.925072
6	8.208938	-1.168245	-4.177944
6	8.103267	0.200535	-4.330457
6	7.988812	-1.384279	4.175126
6	7.829595	-2.637068	3.610079
6	7.885949	2.859724	-2.968050
6	7.783511	3.611823	-1.774203
6	7.525945	-4.243471	1.095537
6	7.406681	-4.303994	-0.315075
6	7.530421	3.868296	1.075513
6	7.380650	3.275450	2.394118
6	7.170312	-3.130297	-2.927687
6	7.055974	-1.964618	-3.794480
6	7.045119	0.982375	4.098180
6	6.873469	-0.461720	4.259995
6	6.835474	0.879931	-4.145161
6	6.737150	2.218111	-3.530011
6	6.541523	-3.079213	3.118499
6	6.398581	-3.924586	1.913127
6	6.479242	3.838755	-1.187243
6	6.356877	3.998082	0.248814
6	6.101249	-4.163299	-0.923193
6	5.986668	-3.595971	-2.253390
6	6.062591	2.911153	2.852682
6	5.897085	1.768542	3.735226
6	5.759843	-1.365312	-3.992613
6	5.651835	0.069826	-4.194494
6	5.555793	-1.023567	4.127648

6	5.389433	-2.357314	3.576915
6	5.429282	2.686805	-3.115738
6	5.305035	3.548346	-1.967097
6	5.077677	-4.072551	1.333826
6	4.931556	-4.247898	-0.088274
6	5.038489	3.945772	0.846346
6	4.891614	3.433952	2.175556
6	4.676002	-3.205838	-2.733958
6	4.561745	-2.104530	-3.640760
6	4.562486	1.243498	3.965187
6	4.391550	-0.156499	4.200956
6	4.338315	0.694760	-4.111968
6	4.228891	2.030945	-3.612500
6	4.052702	-2.803067	3.202763
6	3.897183	-3.705599	2.103818
6	3.989043	3.822134	-1.406721
6	3.859887	4.065193	0.001274
6	3.610788	-4.162363	-0.697043
6	3.486206	-3.678559	-2.043148
6	3.562966	3.124229	2.678984
6	3.400280	2.045065	3.615924
6	3.252200	-1.535085	-3.911687
6	3.143252	-0.125185	-4.190755
6	3.058207	-0.731975	4.161248
6	2.890316	-2.087901	3.694384
6	2.922074	2.561101	-3.266330
6	2.804441	3.504312	-2.176508
6	2.575236	-3.943626	1.554275
6	2.432809	-4.220277	0.140353
6	2.545418	4.067186	0.609683
6	2.400200	3.627530	1.982098
6	2.179927	-3.331350	-2.560103
6	2.065744	-2.267904	-3.537671
6	2.077271	1.540389	3.899546
6	1.907592	0.135535	4.214125
6	1.844598	0.505981	-4.162124
6	1.735558	1.882664	-3.728193
6	1.569451	-2.565898	3.363897
6	1.411395	-3.537124	2.302479
6	1.501030	3.806590	-1.633144
6	1.373305	4.131056	-0.230499
6	1.124234	-4.164975	-0.467952
6	0.997914	-3.753771	-1.846429
6	1.081680	3.336923	2.498111
6	0.921321	2.309131	3.495920
6	0.763450	-1.707936	-3.826363
6	0.653422	-0.316661	-4.179410
6	0.579730	-0.440347	4.190928
6	0.410015	-1.813539	3.800085
6	0.430562	2.421708	-3.399442
6	0.313765	3.420425	-2.372682
6	0.088625	-3.790817	1.762403
6	-0.055932	-4.148226	0.378552
6	0.055933	4.148052	0.380454
6	-0.088625	3.790007	1.764141
6	-0.313765	-3.419337	-2.374249
6	-0.430562	-2.420149	-3.400551
6	-0.410016	1.811795	3.800915
6	-0.579731	0.438424	4.191129
6	-0.653422	0.318577	-4.179264
6	-0.763450	1.709690	-3.825580
6	-0.921321	-2.310735	3.494860
6	-1.081680	-3.338070	2.496580
6	-0.997913	3.754617	-1.844707
6	-1.124233	4.165188	-0.466043
6	-1.373305	-4.130951	-0.232393
6	-1.501029	-3.805842	-1.634889
6	-1.411395	3.536067	2.304099
6	-1.569451	2.564354	3.365071
6	-1.735559	-1.880955	-3.729054

6	-1.844599	-0.504072	-4.162355
6	-1.907593	-0.137469	4.214061
6	-2.077271	-1.542178	3.898839
6	-2.065744	2.269526	-3.536630
6	-2.179926	3.332523	-2.558576
6	-2.400200	-3.628441	1.980435
6	-2.545417	-4.067469	0.607818
6	-2.432808	4.220212	0.142287
6	-2.575235	3.942913	1.556083
6	-2.804441	-3.503315	-2.178113
6	-2.922074	-2.559603	-3.267503
6	-2.890317	2.086206	3.695338
6	-3.058208	0.730066	4.161580
6	-3.143253	0.127107	-4.190695
6	-3.252201	1.536878	-3.910981
6	-3.400280	-2.046724	3.614986
6	-3.562966	-3.125460	2.677552
6	-3.486205	3.679498	-2.041462
6	-3.610787	4.162685	-0.695135
6	-3.859886	-4.065196	-0.000589
6	-3.989043	-3.821490	-1.408472
6	-3.897182	3.704634	2.105515
6	-4.052702	2.801598	3.204046
6	-4.228891	-2.029288	-3.613428
6	-4.338316	-0.692874	-4.112283
6	-4.391551	0.154571	4.201024
6	-4.562487	-1.245317	3.964615
6	-4.561745	2.106200	-3.639793
6	-4.676001	3.207093	-2.732487
6	-4.891614	-3.434952	2.173982
6	-5.038488	-3.946163	0.844538
6	-4.931554	4.247941	-0.086327
6	-5.077676	4.071940	1.335692
6	-5.305035	-3.547445	-1.968722
6	-5.429283	-2.685376	-3.116967
6	-5.389433	2.355673	3.577991
6	-5.555794	1.021674	4.128113
6	-5.651836	-0.067902	-4.194521
6	-5.759844	1.367143	-3.991982
6	-5.897086	-1.770256	3.734413
6	-6.062591	-2.912463	2.851347
6	-5.986666	3.597008	-2.251742
6	-6.101247	4.163727	-0.921285
6	-6.356876	-3.998199	0.246981
6	-6.479241	-3.838213	-1.189002
6	-6.398581	3.923711	1.914924
6	-6.541524	3.077783	3.119906
6	-6.737151	-2.216492	-3.531024
6	-6.835476	-0.878029	-4.145557
6	-6.873470	0.459766	4.260202
6	-7.045120	-0.984255	4.097726
6	-7.055974	1.966360	-3.793575
6	-7.170310	3.131645	-2.926251
6	-7.380650	-3.276551	2.392616
6	-7.530420	-3.868795	1.073740
6	-7.406679	4.304148	-0.313104
6	-7.525944	4.242975	1.097480
6	-7.783511	-3.611013	-1.775857
6	-7.885949	-2.858366	-2.969359
6	-7.829595	2.635412	3.611284
6	-7.988812	1.382364	4.175756
6	-8.103268	-0.198548	-4.330539
6	-8.208939	1.170163	-4.177399
6	-8.348535	-1.603826	3.924331
6	-8.508281	-2.712806	3.120713
6	-8.456574	3.621166	-2.434331
6	-8.571135	4.199836	-1.193314
6	-8.830081	-4.011008	0.417294
6	-8.953274	-3.909227	-0.946367
1	9.945416	3.918854	-1.416883

1	9.730376	4.107236	1.039718
1	9.558641	-4.470689	-0.796853
1	9.359134	-3.433076	-3.032156
1	9.518558	3.091997	2.924490
1	9.234179	1.116113	4.354561
1	9.200356	-1.637774	-4.212185
1	9.013712	0.794467	-4.483204
1	8.997804	-1.035250	4.429610
1	8.716516	-3.257772	3.428224
1	8.888182	2.581203	-3.317973
1	8.535027	-4.211369	1.525967
1	-8.535026	4.210688	1.527898
1	-8.888182	-2.579688	-3.319158
1	-8.716516	3.256200	3.429714
1	-8.997804	1.033221	4.430085
1	-9.013715	-0.792410	-4.483553
1	-9.200358	1.639707	-4.211423
1	-9.234181	-1.118106	4.354039
1	-9.518559	-3.093336	2.923065
1	-9.359132	3.434478	-3.030584
1	-9.558638	4.471072	-0.794808
1	-9.730375	-4.107719	1.037836
1	-9.945416	-3.918208	-1.418678

Nanotube (7,5) u07v03
B3LYP/STO-3G Energy: -6564.639571

6	8.993582	-3.681429	1.873259
6	8.852190	-4.127156	0.582635
6	8.764546	4.230359	0.040790
6	8.652239	3.991169	1.388843
6	8.523861	-3.559158	-2.360958
6	8.376800	-2.689436	-3.420279
6	8.379280	2.072169	3.701504
6	8.250903	0.790915	4.199751
6	8.073350	0.141289	-4.422937
6	7.944509	1.499727	-4.197126
6	7.970063	-2.123998	3.565308
6	7.839493	-3.154473	2.606029
6	7.697096	3.704706	-2.178558
6	7.593052	4.127608	-0.831136
6	7.547555	-4.129324	-0.080211
6	7.393685	-3.891866	-1.504871
6	7.362190	3.668259	1.996366
6	7.236100	2.766889	3.132637
6	7.083696	-2.105442	-3.737907
6	6.938888	-0.748411	-4.263050
6	6.968499	0.112126	4.202267
6	6.839083	-1.335591	3.952013
6	6.669813	2.081009	-3.829458
6	6.555034	3.209611	-2.881690
6	6.523885	-3.497649	2.105863
6	6.381221	-4.017374	0.760160
6	6.291100	4.174274	-0.200311
6	6.179674	3.969563	1.231229
6	6.077357	-3.628513	-2.033448
6	5.924229	-2.747441	-3.178698
6	5.931322	2.264999	3.486048
6	5.799954	0.932202	4.050696
6	5.633721	-0.143126	-4.273634
6	5.499155	1.290658	-4.083224
6	5.518352	-1.868673	3.682148
6	5.364732	-2.993447	2.793644
6	5.243356	3.529490	-2.353678
6	5.114829	4.066134	-1.022902
6	5.057243	-4.091658	0.177825
6	4.904466	-3.934089	-1.237506
6	4.867686	3.741753	1.802657

6	4.743234	2.912536	2.962621
6	4.598038	-2.270159	-3.528031
6	4.452250	-0.974515	-4.115708
6	4.475255	0.333980	4.140065
6	4.336287	-1.082949	4.002027
6	4.175736	1.846037	-3.830071
6	4.048586	3.002486	-2.998186
6	4.037771	-3.373871	2.330951
6	3.886839	-3.964903	1.032933
6	3.799176	4.164994	-0.405534
6	3.679179	4.044065	1.019276
6	3.576333	-3.733234	-1.794551
6	3.424114	-2.928359	-2.976055
6	3.426300	2.457462	3.377499
6	3.295278	1.170935	4.011354
6	3.130934	-0.379490	-4.218728
6	2.994389	1.053195	-4.116511
6	3.015882	-1.657886	3.812977
6	2.868171	-2.845064	3.002843
6	2.736681	3.400759	-2.521173
6	2.613254	4.030906	-1.224698
6	2.564689	-4.092741	0.453677
6	2.411441	-4.014446	-0.983507
6	2.371472	3.866583	1.614750
6	2.248299	3.093056	2.833411
6	2.107658	-2.484603	-3.372518
6	1.962326	-1.206752	-4.039874
6	1.985116	0.580205	4.156216
6	1.846787	-0.859579	4.094684
6	1.686363	1.628850	-3.915114
6	1.557682	2.842203	-3.136742
6	1.552829	-3.250130	2.564882
6	1.401529	-3.916752	1.291082
6	1.310172	4.159298	-0.615983
6	1.190149	4.115473	0.822883
6	1.092579	-3.835835	-1.547849
6	0.941033	-3.096500	-2.776546
6	0.939961	2.652530	3.263930
6	0.809279	1.402521	3.966812
6	0.646771	-0.616140	-4.161738
6	0.508434	0.815262	-4.139147
6	0.529843	-1.439032	3.926736
6	0.382795	-2.665355	3.191391
6	0.246128	3.252847	-2.673180
6	0.121850	3.951735	-1.424439
6	0.077199	-4.058151	0.714031
6	-0.077198	-4.058074	-0.714463
6	-0.121849	3.951582	1.424860
6	-0.246128	3.252560	2.673525
6	-0.382795	-2.665012	-3.191674
6	-0.529843	-1.438611	-3.926888
6	-0.508434	0.814818	4.139233
6	-0.646772	-0.616586	4.161673
6	-0.809280	1.402946	-3.966663
6	-0.939961	2.652880	-3.263648
6	-0.941033	-3.096798	2.776217
6	-1.092579	-3.836002	1.547441
6	-1.190149	4.115562	-0.822445
6	-1.310171	4.159232	0.616426
6	-1.401528	-3.916614	-1.291498
6	-1.552828	-3.249854	-2.565227
6	-1.557682	2.841866	3.137043
6	-1.686363	1.628430	3.915286
6	-1.846787	-0.859140	-4.094774
6	-1.985117	0.580650	-4.156154
6	-1.962327	-1.207185	4.039746
6	-2.107658	-2.484965	3.372254
6	-2.248299	3.093361	-2.833082
6	-2.371471	3.866758	-1.614339
6	-2.411440	-4.014553	0.983080

6	-2.564688	-4.092693	-0.454113
6	-2.613254	4.030775	1.225127
6	-2.736681	3.400488	2.521535
6	-2.868171	-2.844742	-3.003144
6	-3.015883	-1.657478	-3.813152
6	-2.994390	1.052754	4.116621
6	-3.130934	-0.379942	4.218686
6	-3.295278	1.171365	-4.011229
6	-3.426300	2.457825	-3.377238
6	-3.424114	-2.928680	2.975744
6	-3.576333	-3.733429	1.794154
6	-3.679178	4.044177	-1.018846
6	-3.799176	4.164953	0.405977
6	-3.886838	-3.964794	-1.033355
6	-4.037771	-3.373622	-2.331309
6	-4.048587	3.002164	2.998503
6	-4.175737	1.845626	3.830265
6	-4.336288	-1.082520	-4.002140
6	-4.475255	0.334424	-4.140028
6	-4.452251	-0.974956	4.115602
6	-4.598038	-2.270538	3.527789
6	-4.743234	2.912856	-2.962311
6	-4.867685	3.741950	-1.802260
6	-4.904466	-3.934225	1.237088
6	-5.057242	-4.091642	-0.178260
6	-5.114828	4.066027	1.023335
6	-5.243356	3.529239	2.354053
6	-5.364732	-2.993147	-2.793961
6	-5.518352	-1.868278	-3.682344
6	-5.499156	1.290220	4.083357
6	-5.633722	-0.143585	4.273615
6	-5.799954	0.932637	-4.050595
6	-5.931322	2.265374	-3.485807
6	-5.924228	-2.747784	3.178406
6	-6.077357	-3.628735	2.033063
6	-6.179674	3.969700	-1.230807
6	-6.291099	4.174256	0.200755
6	-6.381220	-4.017295	-0.760587
6	-6.523884	-3.497425	-2.106234
6	-6.555034	3.209302	2.882029
6	-6.669814	2.080598	3.829674
6	-6.839084	-1.335167	-3.952151
6	-6.968500	0.112577	-4.202252
6	-6.938888	-0.748869	4.262968
6	-7.083696	-2.105845	3.737683
6	-7.236100	2.767227	-3.132343
6	-7.362189	3.668478	-1.995977
6	-7.393684	-3.892033	1.504457
6	-7.547554	-4.129337	0.079772
6	-7.593051	4.127523	0.831574
6	-7.697097	3.704473	2.178950
6	-7.839493	-3.154194	-2.606362
6	-7.970064	-2.123614	-3.565528
6	-7.944511	1.499276	4.197279
6	-8.073351	0.140815	4.422948
6	-8.250903	0.791365	-4.199663
6	-8.379281	2.072568	-3.701281
6	-8.376800	-2.689807	3.419994
6	-8.523861	-3.559418	2.360581
6	-8.652238	3.991325	-1.388419
6	-8.764545	4.230371	-0.040340
6	-8.852189	-4.127098	-0.583074
6	-8.993581	-3.681231	-1.873650
1	9.990789	-3.591128	2.325967
1	9.742789	-4.400346	0.001975
1	9.752416	4.372226	-0.419111
1	9.556995	3.946905	2.008866
1	9.528384	-3.899976	-2.079350
1	9.266502	-2.350284	-3.966500
1	9.378922	2.515843	3.609687

1	9.151780	0.237759	4.495488
1	9.072472	-0.283173	-4.584968
1	8.845009	2.127379	-4.185217
1	8.981134	-1.785836	3.825740
1	8.700832	3.542845	-2.591862
1	-8.700837	3.542561	2.592234
1	-8.981137	-1.785420	-3.825919
1	-8.845010	2.126929	4.185436
1	-9.072473	-0.283665	4.584933
1	-9.151781	0.238240	-4.495458
1	-9.378922	2.516231	-3.609418
1	-9.266502	-2.350715	3.966252
1	-9.528383	-3.900207	2.078937
1	-9.556993	3.947130	-2.008448
1	-9.752415	4.372190	0.419575
1	-9.742788	-4.400351	-0.002444
1	-9.990789	-3.590881	-2.326348

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B3LYP/STO-3G Energy: -6639.933293

6	9.122314	2.954237	-2.827877
6	9.006151	3.718300	-1.693577
6	8.807920	-4.215901	0.968722
6	8.677239	-4.328950	-0.393829
6	8.712082	3.932291	1.300356
6	8.568210	3.366177	2.548526
6	8.395136	-3.063681	-3.118335
6	8.278013	-1.950758	-3.926471
6	8.241287	0.892105	4.245790
6	8.091108	-0.476026	4.376321
6	8.050948	1.034374	-4.053924
6	7.949911	2.277665	-3.389359
6	7.783327	-3.119608	2.991093
6	7.652013	-3.871278	1.799110
6	7.711208	3.913623	-1.039953
6	7.574253	4.052388	0.398508
6	7.382131	-4.148970	-1.048738
6	7.250811	-3.567563	-2.375951
6	7.271594	2.903995	3.018263
6	7.116081	1.730419	3.874683
6	7.005779	-1.271077	-4.087306
6	6.902052	0.193748	-4.214538
6	6.802796	-1.110836	4.183351
6	6.658504	-2.441318	3.558071
6	6.646699	2.761882	-2.980813
6	6.531007	3.611243	-1.812262
6	6.339211	-4.055964	1.216736
6	6.207450	-4.222956	-0.217598
6	6.261736	3.956312	0.990624
6	6.112657	3.401144	2.325026
6	5.947720	-3.149181	-2.831158
6	5.827272	-2.003751	-3.717483
6	5.802964	1.170261	4.054783
6	5.646514	-0.262095	4.240472
6	5.593743	0.802463	-4.077463
6	5.470255	2.120186	-3.505507
6	5.334755	-2.864469	3.146186
6	5.177888	-3.721654	1.998515
6	5.217065	3.856230	-1.255153
6	5.082159	4.068221	0.155153
6	4.890025	-4.125648	-0.812725
6	4.758835	-3.618623	-2.145126
6	4.785657	3.051458	2.798502
6	4.630847	1.952608	3.700697
6	4.510834	-1.424283	-3.942476
6	4.395460	-0.017120	-4.172360
6	4.312778	-0.841417	4.153485

6	4.157656	-2.170021	3.648219
6	4.156468	2.630739	-3.142603
6	4.032885	3.536053	-2.037576
6	3.851774	-3.952165	1.442594
6	3.710171	-4.195775	0.036093
6	3.759453	4.038211	0.758568
6	3.612582	3.564913	2.107185
6	3.442261	-3.259629	-2.646412
6	3.320296	-2.177604	-3.587845
6	3.302863	1.425700	3.966392
6	3.145752	0.018814	4.238667
6	3.086891	0.611417	-4.123747
6	2.969097	1.968693	-3.645314
6	2.832940	-2.655762	3.305126
6	2.680567	-3.593337	2.215480
6	2.720908	3.831140	-1.496706
6	2.586514	4.123506	-0.086261
6	2.394988	-4.151591	-0.569356
6	2.263087	-3.712112	-1.942485
6	2.295274	3.259361	2.617423
6	2.142120	2.198841	3.592445
6	2.016634	-1.619641	-3.865298
6	1.901130	-0.211278	-4.177806
6	1.827177	-0.567626	4.208694
6	1.670753	-1.938903	3.772250
6	1.666522	2.497446	-3.313838
6	1.543407	3.469608	-2.250966
6	1.366181	-3.851832	1.676115
6	1.222993	-4.171379	0.274299
6	1.273571	4.117263	0.518108
6	1.128924	3.717505	1.896467
6	0.954476	-3.371622	-2.455263
6	0.831354	-2.342294	-3.455631
6	0.821342	1.681575	3.876126
6	0.663873	0.295361	4.227092
6	0.596298	0.416380	-4.153345
6	0.479132	1.794012	-3.758584
6	0.348076	-2.433906	3.447039
6	0.194735	-3.427087	2.420408
6	0.230279	3.776761	-1.715968
6	0.095687	4.140396	-0.332735
6	-0.095687	-4.140394	-0.332760
6	-0.230279	-3.776750	-1.715991
6	-0.194735	3.427072	2.420428
6	-0.348075	2.433885	3.447053
6	-0.479132	-1.793988	-3.758594
6	-0.596298	-0.416354	-4.153347
6	-0.663873	-0.295387	4.227090
6	-0.821342	-1.681599	3.876116
6	-0.831354	2.342315	-3.455617
6	-0.954476	3.371638	-2.455243
6	-1.128924	-3.717516	1.896445
6	-1.273571	-4.117266	0.518083
6	-1.222993	4.171377	0.274324
6	-1.366181	3.851821	1.676138
6	-1.543407	-3.469594	-2.250986
6	-1.666522	-2.497426	-3.313852
6	-1.670752	1.938880	3.772262
6	-1.827177	0.567600	4.208697
6	-1.901130	0.211304	-4.177805
6	-2.016634	1.619665	-3.865288
6	-2.142120	-2.198863	3.592432
6	-2.295274	-3.259377	2.617404
6	-2.263088	3.712124	-1.942462
6	-2.394989	4.151595	-0.569331
6	-2.586514	-4.123506	-0.086285
6	-2.720908	-3.831130	-1.496729
6	-2.680566	3.593323	2.215502
6	-2.832940	2.655742	3.305142
6	-2.969097	-1.968670	-3.645325

6	-3.086891	-0.611392	-4.123750
6	-3.145752	-0.018840	4.238667
6	-3.302863	-1.425724	3.966384
6	-3.320297	2.177625	-3.587832
6	-3.442261	3.259645	-2.646391
6	-3.612582	-3.564926	2.107164
6	-3.759453	-4.038215	0.758545
6	-3.710171	4.195775	0.036119
6	-3.851773	3.952156	1.442618
6	-4.032885	-3.536040	-2.037597
6	-4.156468	-2.630719	-3.142618
6	-4.157656	2.169998	3.648233
6	-4.312778	0.841391	4.153491
6	-4.395460	0.017145	-4.172360
6	-4.510835	1.424307	-3.942466
6	-4.630847	-1.952631	3.700687
6	-4.785657	-3.051476	2.798484
6	-4.758835	3.618635	-2.145103
6	-4.890026	4.125652	-0.812700
6	-5.082160	-4.068221	0.155130
6	-5.217065	-3.856221	-1.255176
6	-5.177887	3.721641	1.998538
6	-5.334755	2.864450	3.146203
6	-5.470255	-2.120164	-3.505519
6	-5.593742	-0.802438	-4.077469
6	-5.646514	0.262069	4.240475
6	-5.802964	-1.170286	4.054777
6	-5.827272	2.003772	-3.717470
6	-5.947721	3.149198	-2.831138
6	-6.112657	-3.401159	2.325007
6	-6.261736	-3.956317	0.990601
6	-6.207450	4.222957	-0.217572
6	-6.339210	4.055956	1.216761
6	-6.531007	-3.611231	-1.812283
6	-6.646698	-2.761864	-2.980831
6	-6.658504	2.441296	3.558086
6	-6.802796	1.110811	4.183358
6	-6.902052	-0.193724	-4.214543
6	-7.005780	1.271101	-4.087300
6	-7.116081	-1.730443	3.874674
6	-7.271594	-2.904014	3.018247
6	-7.250811	3.567577	-2.375930
6	-7.382131	4.148976	-1.048713
6	-7.574253	-4.052389	0.398484
6	-7.711209	-3.913615	-1.039976
6	-7.652013	3.871267	1.799135
6	-7.783327	3.119591	2.991113
6	-7.949910	-2.277647	-3.389376
6	-8.050946	-1.034353	-4.053939
6	-8.091108	0.475999	4.376324
6	-8.241287	-0.892131	4.245785
6	-8.278013	1.950784	-3.926462
6	-8.395136	3.063702	-3.118319
6	-8.568210	-3.366194	2.548507
6	-8.712082	-3.932301	1.300334
6	-8.677239	4.328954	-0.393801
6	-8.807919	4.215897	0.968748
6	-9.006151	-3.718288	-1.693600
6	-9.122313	-2.954220	-2.827898
1	10.111377	2.733284	-3.252665
1	9.908896	4.115479	-1.211630
1	9.800835	-4.253472	1.438005
1	9.572230	-4.462529	-1.015218
1	9.716831	4.173944	0.930764
1	9.460550	3.164766	3.155253
1	9.389094	-3.488564	-2.928423
1	9.181906	-1.509054	-4.365701
1	9.247960	1.327745	4.284352
1	8.982487	-1.101041	4.517012
1	9.052740	0.622170	-4.229818

1	8.795438	-2.874835	3.337808
1	-8.795436	2.874817	3.337828
1	-9.052740	-0.622150	-4.229832
1	-8.982487	1.101013	4.517019
1	-9.247960	-1.327772	4.284345
1	-9.181906	1.509086	-4.365699
1	-9.389094	3.488585	-2.928406
1	-9.460550	-3.164788	3.155237
1	-9.716832	-4.173954	0.930742
1	-9.572230	4.462539	-1.015190
1	-9.800834	4.253467	1.438033
1	-9.908896	-4.115469	-1.211655
1	-10.111375	-2.733267	-3.252686

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B3LYP/STO-3G Energy: -6715.230940

6	9.223828	-2.215364	3.401852
6	9.081885	-3.250395	2.499696
6	8.917201	3.722586	-2.126097
6	8.811708	4.188198	-0.829647
6	8.733268	-4.228694	-0.329223
6	8.572232	-4.003658	-1.689404
6	8.561376	3.682320	2.131914
6	8.446952	2.812528	3.211324
6	8.240074	-2.053135	-3.966169
6	8.102479	-0.752870	-4.448346
6	8.192991	-0.032694	4.121247
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6	7.847987	2.166991	-3.795113
6	7.748324	3.213209	-2.823789
6	7.782586	-3.599062	1.950865
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6	7.534615	4.216029	-0.140634
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6	7.282892	-3.671121	-2.241802
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6	7.183362	2.221982	3.560776
6	7.068017	0.826994	4.069489
6	6.837884	-0.074944	-4.409414
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6	6.764888	-1.968832	3.537384
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6	6.454691	3.551513	-2.286458
6	6.349973	4.080226	-0.940408
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6	6.133146	-3.939362	-1.422728
6	6.122301	3.713162	1.868159
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6	5.813997	-2.223340	-3.668182
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6	5.745265	0.222212	4.100545
6	5.598991	-1.193603	3.892328
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6	5.290724	-3.450066	2.168476
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6	5.035683	4.160327	-0.322645
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6	4.682137	2.363048	3.410659
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6	4.340287	-0.290713	-4.271911
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B3LYP/STO-3G Energy: -6790.530019

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1	-9.379724	3.410918	-3.082842
1	-9.433140	-3.332796	3.000575
1	-9.196407	-1.341268	4.409058
1	-9.224616	1.512586	-4.039537
1	-9.024362	0.781830	4.284648
1	9.024356	-0.781665	4.284714

1	9.224611	-1.512741	-4.039520
1	9.196399	1.341438	4.409049
1	9.433138	3.332898	3.000470
1	9.379725	-3.411026	-3.082719
1	9.610852	-4.409468	-0.856066
1	9.628393	4.352748	1.112067
1	9.870440	4.120581	-1.317450
1	9.812693	-4.290165	1.272701
1	10.041339	-2.889595	3.294766
1	10.059805	3.009665	-3.135231
1	10.265976	0.799513	-4.221029

Nanotube (7,5) u07v07
B3LYP/STO-3G Energy: -6865.828727

6	9.449198	0.174150	-4.024864
6	9.319436	1.520315	-3.754945
6	9.095093	-2.235183	3.715571
6	8.985036	-3.280753	2.820995
6	8.985662	3.774442	-1.782923
6	8.823826	4.254296	-0.492045
6	8.735374	-4.308581	-0.002672
6	8.626111	-4.088000	-1.370193
6	8.471955	3.694482	2.450761
6	8.320998	2.806655	3.512542
6	8.394980	-2.067222	-3.570384
6	8.287617	-0.702862	-3.975969
6	8.038771	-0.049399	4.389692
6	7.929953	-1.437187	4.064820
6	8.023333	2.107955	-3.454499
6	7.867279	3.229416	-2.519039
6	7.705854	-3.637453	2.231788
6	7.590806	-4.164771	0.863102
6	7.529831	4.252937	0.147119
6	7.360688	4.017097	1.595164
6	7.365014	-3.738290	-1.970185
6	7.260695	-2.778601	-3.102581
6	7.048094	2.209350	3.808457
6	6.915820	0.809614	4.301861
6	6.986000	-0.084621	-4.027862
6	6.856944	1.341002	-3.791331
6	6.632861	-1.988618	3.762856
6	6.523283	-3.115598	2.856480
6	6.550722	3.554995	-2.038995
6	6.382798	4.093971	-0.702617
6	6.295468	-4.188238	0.235716
6	6.183019	-3.996512	-1.197155
6	6.046801	3.717463	2.095769
6	5.888411	2.828954	3.229015
6	5.944612	-2.256025	-3.432427
6	5.812537	-0.921957	-3.953640
6	5.593100	0.203939	4.284180
6	5.455184	-1.212008	4.072291
6	5.530442	1.895648	-3.579709
6	5.377071	3.038531	-2.728286
6	5.208452	-3.482245	2.355444
6	5.093695	-4.059817	1.047421
6	5.043529	4.169798	-0.134762
6	4.874865	4.019659	1.283399
6	4.863541	-3.763793	-1.776627
6	4.748925	-2.920786	-2.939903
6	4.553019	2.347376	3.568052
6	4.408426	1.035403	4.150924
6	4.495487	-0.318470	-4.075021
6	4.360464	1.116042	-3.929389
6	4.140697	-1.785500	3.838938
6	4.022716	-2.962447	3.001230
6	4.053859	3.436040	-2.300206

6	3.888766	4.049579	-0.993454
6	3.791904	-4.178199	0.432395
6	3.680933	-4.064091	-1.013931
6	3.554474	3.820974	1.827189
6	3.395178	2.997783	3.018308
6	3.448338	-2.452836	-3.352086
6	3.324057	-1.143618	-3.971036
6	3.100217	0.436010	4.231863
6	2.966770	-1.006213	4.116604
6	3.050026	1.690624	-3.760475
6	2.898318	2.890606	-2.962833
6	2.723398	-3.365209	2.525451
6	2.609231	-4.014009	1.236332
6	2.569112	4.164714	-0.428405
6	2.401109	4.084859	1.005361
6	2.379151	-3.862022	-1.606269
6	2.263094	-3.078605	-2.812223
6	2.075577	2.536254	3.383815
6	1.926615	1.258133	4.035029
6	2.012624	-0.544908	-4.110609
6	1.876449	0.888904	-4.047859
6	1.655664	-1.584338	3.899763
6	1.533841	-2.798859	3.132231
6	1.570832	3.300208	-2.542004
6	1.406570	3.980513	-1.280538
6	1.299536	-4.148441	0.622833
6	1.186099	-4.111705	-0.816516
6	1.069201	3.904522	1.556783
6	0.907027	3.155871	2.783477
6	0.952373	-2.631554	-3.248808
6	0.830141	-1.367622	-3.947195
6	0.607005	0.665069	4.149880
6	0.473069	-0.778938	4.126553
6	0.559148	1.475691	-3.911656
6	0.409192	2.723238	-3.181770
6	0.228043	-3.229463	2.679988
6	0.113934	-3.950230	1.422580
6	0.083676	4.137096	-0.722930
6	-0.083677	4.137083	0.723011
6	-0.113936	-3.950203	-1.422669
6	-0.228044	-3.229412	-2.680063
6	-0.409191	2.723178	3.181823
6	-0.559147	1.475614	3.911683
6	-0.473068	-0.778857	-4.126577
6	-0.607004	0.665151	-4.149872
6	-0.830139	-1.367700	3.947159
6	-0.952372	-2.631616	3.248746
6	-0.907027	3.155924	-2.783415
6	-1.069202	3.904550	-1.556707
6	-1.186101	-4.111719	0.816424
6	-1.299539	-4.148428	-0.622925
6	-1.406571	3.980488	1.280616
6	-1.570832	3.300159	2.542070
6	-1.533843	-2.798797	-3.132297
6	-1.655665	-1.584260	-3.899805
6	-1.876447	0.888824	4.047875
6	-2.012621	-0.544989	4.110594
6	-1.926615	1.258213	-4.035008
6	-2.075577	2.536319	-3.383767
6	-2.263093	-3.078658	2.812153
6	-2.379151	-3.862050	1.606183
6	-2.401110	4.084876	-1.005280
6	-2.569114	4.164703	0.428487
6	-2.609233	-4.013982	-1.236421
6	-2.723401	-3.365157	-2.525527
6	-2.898317	2.890548	2.962892
6	-3.050024	1.690550	3.760510
6	-2.966771	-1.006130	-4.116633
6	-3.100218	0.436096	-4.231861
6	-3.324052	-1.143697	3.971012

6	-3.448335	-2.452900	3.352032
6	-3.395178	2.997841	-3.018250
6	-3.554474	3.821007	-1.827113
6	-3.680934	-4.064105	1.013844
6	-3.791906	-4.178185	-0.432484
6	-3.888767	4.049556	0.993535
6	-4.053859	3.435992	2.300276
6	-4.022720	-2.962384	-3.001295
6	-4.140700	-1.785421	-3.838981
6	-4.360461	1.115963	3.929416
6	-4.495482	-0.318552	4.075019
6	-4.408426	1.035488	-4.150910
6	-4.553019	2.347448	-3.568009
6	-4.748922	-2.920843	2.939843
6	-4.863540	-3.763823	1.776549
6	-4.874866	4.019680	-1.283318
6	-5.043531	4.169789	0.134847
6	-5.093698	-4.059788	-1.047505
6	-5.208456	-3.482192	-2.355517
6	-5.377070	3.038473	2.728350
6	-5.530440	1.895574	3.579752
6	-5.455187	-1.211923	-4.072321
6	-5.593102	0.204029	-4.284183
6	-5.812530	-0.922039	3.953631
6	-5.944607	-2.256095	3.432388
6	-5.888412	2.829021	-3.228962
6	-6.046802	3.717503	-2.095695
6	-6.183020	-3.996529	1.197076
6	-6.295470	-4.188225	-0.235800
6	-6.382799	4.093947	0.702701
6	-6.550723	3.554946	2.039069
6	-6.523287	-3.115533	-2.856543
6	-6.632865	-1.988536	-3.762898
6	-6.856939	1.340922	3.791369
6	-6.985994	-0.084706	4.027877
6	-6.915821	0.809706	-4.301852
6	-7.048095	2.209432	-3.808419
6	-7.260691	-2.778665	3.102537
6	-7.365012	-3.738324	1.970115
6	-7.360689	4.017122	-1.595082
6	-7.529833	4.252929	-0.147031
6	-7.590809	-4.164744	-0.863184
6	-7.705859	-3.637398	-2.231858
6	-7.867279	3.229356	2.519109
6	-8.023331	2.107880	3.454553
6	-7.929957	-1.437097	-4.064849
6	-8.038774	-0.049303	-4.389697
6	-8.287609	-0.702949	3.975982
6	-8.394975	-2.067298	3.570364
6	-8.320999	2.806730	-3.512491
6	-8.471956	3.694529	-2.450685
6	-8.626110	-4.088021	1.370117
6	-8.735376	-4.308572	0.002591
6	-8.823827	4.254270	0.492132
6	-8.985664	3.774390	1.783002
6	-8.985043	-3.280683	-2.821055
6	-9.095098	-2.235097	-3.715612
6	-9.319430	1.520233	3.755000
6	-9.449189	0.174063	4.024901
1	10.445851	-0.273563	-4.141365
1	10.220530	2.140212	-3.662116
1	10.084400	-1.908798	4.064897
1	9.894533	-3.782665	2.466307
1	9.999280	3.677130	-2.191978
1	9.713229	4.524066	0.091940
1	9.731979	-4.445713	0.435767
1	9.540555	-4.053988	-1.976506
1	9.481630	4.025144	2.175685
1	9.217200	2.460883	4.043837
1	9.401627	-2.466568	-3.390520

1	9.047630	0.377162	4.462942
1	-9.047628	0.377259	-4.462944
1	-9.401645	-2.466634	3.390463
1	-9.217201	2.460972	-4.043794
1	-9.481629	4.025181	-2.175600
1	-9.540552	-4.054025	1.976433
1	-9.731983	-4.445699	-0.435851
1	-9.713231	4.524048	-0.091849
1	-9.999284	3.677062	2.192054
1	-9.894540	-3.782600	-2.466373
1	-10.084400	-1.908710	-4.064937
1	-10.220527	2.140129	3.662187
1	-10.445844	-0.273649	4.141402

Nanotube (7,5) u07v08
B3LYP/STO-3G Energy: -6941.127044

6	-9.478696	-4.072452	-0.862644
6	-9.347051	-4.154605	0.507091
6	-9.273391	4.042394	-1.207097
6	-9.152949	3.447283	-2.446318
6	-9.039401	-2.817424	3.190395
6	-8.899395	-1.689697	3.983864
6	-8.860452	0.983077	-4.160025
6	-8.726330	-0.392609	-4.297322
6	-8.603447	1.305236	4.196328
6	-8.474820	2.561550	3.611855
6	-8.444967	-3.034503	-2.911001
6	-8.322537	-3.775295	-1.698100
6	-8.219192	4.149743	1.078633
6	-8.110548	4.194258	-0.345207
6	-8.053261	-3.987870	1.152191
6	-7.909445	-3.368169	2.474678
6	-7.865188	2.989990	-2.941405
6	-7.729651	1.804281	-3.800741
6	-7.616650	-1.046501	4.146490
6	-7.475018	0.415624	4.289762
6	-7.452325	-1.039337	-4.115054
6	-7.322599	-2.377873	-3.479208
6	-7.208762	3.024680	3.112041
6	-7.090746	3.863501	1.886858
6	-7.016601	-3.959564	-1.114390
6	-6.884543	-4.094546	0.324300
6	-6.810691	4.066469	-0.955520
6	-6.691004	3.481161	-2.277360
6	-6.600453	-2.962824	2.913171
6	-6.455015	-1.805934	3.776908
6	-6.423944	1.227541	-3.986023
6	-6.285811	-0.204543	-4.168355
6	-6.171616	1.000912	4.131217
6	-6.037005	2.327332	3.563537
6	-5.998492	-2.806604	-3.060137
6	-5.849553	-3.649991	-1.904635
6	-5.770858	4.025279	1.297279
6	-5.635332	4.186115	-0.125509
6	-5.559803	-4.005531	0.914393
6	-5.416990	-3.473134	2.236965
6	-5.369746	3.113644	-2.760141
6	-5.235735	2.000530	-3.654185
6	-5.126399	-1.251213	3.996484
6	-4.984330	0.159937	4.215523
6	-4.955105	-0.800166	-4.093198
6	-4.815177	-2.137341	-3.577118
6	-4.709592	2.802363	3.185230
6	-4.580302	3.703301	2.067117
6	-4.526647	-3.895824	-1.352342
6	-4.386665	-4.119709	0.070337
6	-4.318962	4.129743	-0.739497

6	-4.192174	3.624931	-2.091624
6	-4.099147	-3.135501	2.731287
6	-3.955728	-2.028947	3.660194
6	-3.923601	1.460317	-3.928128
6	-3.787115	0.035921	-4.190147
6	-3.673687	0.761178	4.165076
6	-3.538974	2.125546	3.674895
6	-3.504355	-2.632013	-3.232232
6	-3.361302	-3.562400	-2.124617
6	-3.275457	3.958581	1.508863
6	-3.146345	4.218699	0.085007
6	-3.076300	-4.078362	0.668830
6	-2.933909	-3.613361	2.034179
6	-2.886879	3.292088	-2.603783
6	-2.754299	2.216001	-3.563527
6	-2.646387	-1.488482	3.919549
6	-2.505203	-0.079018	4.211863
6	-2.474897	-0.564732	-4.149558
6	-2.333290	-1.928687	-3.700915
6	-2.228363	2.621213	3.323523
6	-2.095962	3.579268	2.253478
6	-2.044862	-3.823914	-1.581750
6	-1.902224	-4.125877	-0.179754
6	-1.834459	4.179311	-0.529232
6	-1.705171	3.752329	-1.900089
6	-1.613264	-3.285619	2.538323
6	-1.469623	-2.241330	3.521504
6	-1.435049	1.681352	-3.852581
6	-1.296800	0.284525	-4.189252
6	-1.184374	0.525060	4.180004
6	-1.047034	1.903399	3.770099
6	-1.011993	-2.440413	-3.381205
6	-0.869313	-3.432596	-2.336956
6	-0.780151	3.863865	1.709225
6	-0.651886	4.211756	0.307797
6	-0.583375	-4.116102	0.422286
6	-0.441153	-3.730394	1.814113
6	-0.393273	3.449106	-2.432894
6	-0.261571	2.423957	-3.454946
6	-0.155099	-1.718076	3.819172
6	-0.014510	-0.319762	4.193214
6	0.014511	-0.319153	-4.193259
6	0.155100	-1.717520	-3.819419
6	0.261571	2.423455	3.455297
6	0.393272	3.448752	2.433394
6	0.441153	-3.730131	-1.814653
6	0.583375	-4.116042	-0.422882
6	0.651884	4.211801	-0.307186
6	0.780149	3.864115	-1.708664
6	0.869313	-3.432936	2.336459
6	1.011994	-2.440904	3.380851
6	1.047034	1.903947	-3.769822
6	1.184375	0.525667	-4.179926
6	1.296801	0.283917	4.189292
6	1.435050	1.680792	3.852824
6	1.469624	-2.240818	-3.521828
6	1.613264	-3.285251	-2.538799
6	1.705170	3.752053	1.900632
6	1.834457	4.179236	0.529839
6	1.902223	-4.125905	0.179155
6	2.044861	-3.824146	1.581195
6	2.095961	3.579597	-2.252958
6	2.228362	2.621696	-3.323142
6	2.333291	-1.929225	3.700634
6	2.474899	-0.565334	4.149475
6	2.505204	-0.078406	-4.211871
6	2.646388	-1.487913	-3.919762
6	2.754300	2.215483	3.563846
6	2.886878	3.291711	2.604259
6	2.933909	-3.613067	-2.034702

6	3.076299	-4.078268	-0.669421
6	3.146343	4.218715	-0.084395
6	3.275456	3.958804	-1.508288
6	3.361302	-3.562711	2.124100
6	3.504355	-2.632484	3.231849
6	3.538975	2.126080	-3.674584
6	3.673689	0.761783	-4.164961
6	3.787117	0.035313	4.190148
6	3.923603	1.459747	3.928336
6	3.955729	-2.028415	-3.660485
6	4.099148	-3.135105	-2.731740
6	4.192173	3.624631	2.092150
6	4.318960	4.129642	0.740096
6	4.386664	-4.119704	-0.070935
6	4.526646	-3.896025	1.351777
6	4.580301	3.703605	-2.066579
6	4.709592	2.802828	-3.184822
6	4.815178	-2.137861	3.576805
6	4.955107	-0.800760	4.093077
6	4.984332	0.160550	-4.215495
6	5.126400	-1.250632	-3.996660
6	5.235736	2.000000	3.654471
6	5.369745	3.113246	2.760591
6	5.416990	-3.472812	-2.237467
6	5.559802	-4.005403	-0.914974
6	5.635330	4.186105	0.126117
6	5.770856	4.025474	-1.296695
6	5.849552	-3.650273	1.904106
6	5.998491	-2.807050	3.059728
6	6.037005	2.327852	-3.563196
6	6.171618	1.001513	-4.131065
6	6.285813	-0.205147	4.168317
6	6.423946	1.226963	3.986193
6	6.455016	-1.805386	-3.777164
6	6.600453	-2.962403	-2.913598
6	6.691004	3.480836	2.277863
6	6.810690	4.066340	0.956110
6	6.884542	-4.094506	-0.324894
6	7.016600	-3.959732	1.113816
6	7.090744	3.863783	-1.886298
6	7.208762	3.025135	-3.111598
6	7.322599	-2.378380	3.478860
6	7.452327	-1.039934	4.114894
6	7.475020	0.416248	-4.289692
6	7.616651	-1.045898	-4.146633
6	7.729653	1.803730	3.800993
6	7.865188	2.989568	2.941834
6	7.909444	-3.367814	-2.475164
6	8.053260	-3.987711	-1.152769
6	8.110546	4.194219	0.345815
6	8.219189	4.149914	-1.078032
6	8.322536	-3.775550	1.697553
6	8.444967	-3.034932	2.910561
6	8.474820	2.562077	-3.611476
6	8.603449	1.305847	-4.196129
6	8.726332	-0.393234	4.297251
6	8.860454	0.982473	4.160150
6	8.899395	-1.689118	-3.984102
6	9.039402	-2.816963	-3.190799
6	9.152949	3.446931	2.446813
6	9.273391	4.042226	1.207680
6	9.347049	-4.154542	-0.507693
6	9.478694	-4.072588	0.862054
1	-10.475058	-4.091542	-1.325598
1	-10.246068	-4.243971	1.130495
1	-10.266825	4.280980	-0.802555
1	-10.058230	3.218702	-3.023477
1	-10.045508	-3.208487	2.992234
1	-9.797822	-1.211662	4.395205
1	-9.865197	1.424134	-4.179430

1	-9.629686	-1.004165	-4.419574
1	-9.606630	0.935882	4.444829
1	-9.381314	3.148239	3.414152
1	-9.456576	-2.777885	-3.250793
1	-9.227105	4.094298	1.509679
1	9.227101	4.094539	-1.509086
1	9.456575	-2.778368	3.250393
1	9.381315	3.148736	-3.413687
1	9.606631	0.936529	-4.444684
1	9.629688	-1.004807	4.419413
1	9.865203	1.423527	4.179610
1	9.797823	-1.211023	-4.395373
1	10.045510	-3.208055	-2.992693
1	10.058230	3.218261	3.023936
1	10.266827	4.280863	0.803168
1	10.246067	-4.243819	-1.131108
1	10.475056	-4.091746	1.325005

Nanotube (7,5) u07v09
B3LYP/STO-3G Energy: -7016.424961

6	9.636632	3.593913	-1.910838
6	9.517460	4.027200	-0.608196
6	9.304529	-4.336904	-0.165828
6	9.181714	-4.077413	-1.515005
6	9.212880	3.428337	2.329438
6	9.063514	2.544071	3.385420
6	8.912664	-2.128104	-3.799917
6	8.799049	-0.831846	-4.283816
6	8.726503	-0.292272	4.356985
6	8.574179	-1.653533	4.114660
6	8.570372	2.081641	-3.618956
6	8.468992	3.110219	-2.637177
6	8.270507	-3.834523	2.075853
6	8.147327	-4.241013	0.712723
6	8.226149	4.052048	0.064001
6	8.084423	3.794861	1.500807
6	7.896131	-3.738319	-2.104109
6	7.771608	-2.810503	-3.236891
6	7.772502	1.984056	3.712950
6	7.611366	0.610358	4.226159
6	7.536102	-0.137743	-4.267825
6	7.432621	1.320298	-3.996023
6	7.296028	-2.208662	3.757894
6	7.153709	-3.331287	2.790042
6	7.170430	3.460611	-2.115215
6	7.052201	3.962356	-0.758725
6	6.843567	-4.251725	0.096687
6	6.720521	-4.022720	-1.330596
6	6.773354	3.536941	2.034742
6	6.618827	2.642436	3.167118
6	6.473514	-2.278191	-3.558492
6	6.356515	-0.938189	-4.101506
6	6.298368	0.025427	4.230896
6	6.139327	-1.399998	4.022948
6	6.119310	1.865220	-3.696381
6	5.992789	2.978845	-2.794809
6	5.826531	-3.616691	2.268812
6	5.674801	-4.133826	0.935454
6	5.731532	4.048584	-0.159679
6	5.591993	3.874981	1.255427
6	5.401085	-3.766977	-1.884518
6	5.276623	-2.918590	-3.033103
6	5.284447	2.183707	3.527541
6	5.124253	0.879184	4.102414
6	5.036190	-0.320064	-4.175554
6	4.921463	1.105756	-4.019501
6	4.801521	-1.934110	3.786108

6	4.648065	-3.087897	2.937134
6	4.677952	3.379640	-2.317903
6	4.552780	3.961301	-1.000088
6	4.353010	-4.212483	0.334047
6	4.221094	-4.068267	-1.100435
6	4.272808	3.695831	1.825559
6	4.121569	2.867793	3.007769
6	3.969770	-2.443407	-3.430341
6	3.853564	-1.133345	-4.049602
6	3.804065	0.306717	4.215742
6	3.645127	-1.135142	4.093778
6	3.620612	1.695402	-3.808718
6	3.500989	2.880133	-2.975497
6	3.333810	-3.456145	2.470423
6	3.186690	-4.068284	1.160519
6	3.246472	4.096046	-0.405273
6	3.108778	3.997853	1.034594
6	2.916145	-3.854770	-1.674158
6	2.792006	-3.059201	-2.878246
6	2.807019	2.433656	3.404087
6	2.648584	1.149452	4.051057
6	2.551839	-0.519893	-4.161052
6	2.435651	0.916328	-4.077942
6	2.324975	-1.683164	3.889706
6	2.168205	-2.880316	3.100658
6	2.193681	3.293737	-2.512143
6	2.066936	3.944530	-1.232483
6	1.870260	-4.162648	0.563540
6	1.734496	-4.096510	-0.869648
6	1.787902	3.830343	1.611429
6	1.637718	3.076546	2.830427
6	1.479421	-2.592668	-3.288356
6	1.360462	-1.329611	-3.974116
6	1.318990	0.578955	4.182958
6	1.158122	-0.855211	4.143979
6	1.125168	1.515738	-3.894546
6	1.006130	2.742184	-3.138238
6	0.842539	-3.271969	2.654148
6	0.694644	-3.959888	1.388580
6	0.752093	4.108817	-0.641986
6	0.615716	4.092793	0.802107
6	0.421238	-3.913897	-1.455099
6	0.296466	-3.185532	-2.704847
6	0.317809	2.668646	3.259169
6	0.160854	1.417633	3.983575
6	0.057581	-0.724180	-4.130039
6	-0.057581	0.724582	-4.129970
6	-0.160854	-1.418023	3.983438
6	-0.317809	-2.668965	3.258911
6	-0.296465	3.185796	-2.704540
6	-0.421238	3.914039	-1.454720
6	-0.615716	-4.092873	0.801711
6	-0.752092	-4.108755	-0.642384
6	-0.694644	3.959751	1.388963
6	-0.842539	3.271709	2.654465
6	-1.006130	-2.741877	-3.138503
6	-1.125169	-1.515358	-3.894692
6	-1.158123	0.854806	4.144061
6	-1.318990	-0.579364	4.182902
6	-1.360462	1.329999	-3.973988
6	-1.479421	2.592989	-3.288106
6	-1.637719	-3.076824	2.830130
6	-1.787902	-3.830503	1.611057
6	-1.734495	4.096595	-0.869252
6	-1.870260	4.162593	0.563944
6	-2.066936	-3.944410	-1.232865
6	-2.193681	-3.293492	-2.512461
6	-2.168206	2.880012	3.100936
6	-2.324975	1.682784	3.889867
6	-2.435652	-0.915930	-4.078029

6	-2.551839	0.520298	-4.161001
6	-2.648584	-1.149848	4.050945
6	-2.807019	-2.433990	3.403851
6	-2.792006	3.059483	-2.877951
6	-2.916145	3.854935	-1.673785
6	-3.108778	-3.997957	1.034207
6	-3.246472	-4.096008	-0.405670
6	-3.186690	4.068170	1.160912
6	-3.333810	3.455903	2.470757
6	-3.500989	-2.879842	-2.975774
6	-3.620612	-1.695030	-3.808880
6	-3.645127	1.134742	4.093886
6	-3.804066	-0.307129	4.215710
6	-3.853564	1.133740	-4.049492
6	-3.969770	2.443743	-3.430105
6	-4.121569	-2.868088	3.007492
6	-4.272808	-3.696011	1.825201
6	-4.221094	4.068377	-1.100042
6	-4.353009	4.212452	0.334455
6	-4.552780	-3.961205	-1.000472
6	-4.677952	-3.379414	-2.318230
6	-4.648065	3.087610	2.937431
6	-4.801522	1.933740	3.786293
6	-4.921464	-1.105363	-4.019605
6	-5.036190	0.320472	-4.175521
6	-5.124253	-0.879585	4.102328
6	-5.284447	-2.184052	3.527330
6	-5.276623	2.918888	-3.032821
6	-5.401084	3.767164	-1.884154
6	-5.591993	-3.875106	1.255051
6	-5.731532	-4.048570	-0.160071
6	-5.674800	4.133737	0.935853
6	-5.826530	3.616469	2.269160
6	-5.992789	-2.978572	-2.795096
6	-6.119310	-1.864859	-3.696558
6	-6.139327	1.399605	4.023080
6	-6.298369	-0.025840	4.230891
6	-6.356515	0.938590	-4.101413
6	-6.473514	2.278540	-3.558271
6	-6.618827	-2.642747	3.166863
6	-6.773354	-3.537142	2.034399
6	-6.720520	4.022853	-1.330207
6	-6.843566	4.251718	0.097098
6	-7.052201	-3.962283	-0.759109
6	-7.170430	-3.460404	-2.115550
6	-7.153709	3.331015	2.790362
6	-7.296029	2.208295	3.758103
6	-7.432622	-1.319908	-3.996149
6	-7.536102	0.138160	-4.267809
6	-7.611367	-0.610771	4.226098
6	-7.772503	-1.984419	3.712758
6	-7.771608	2.810821	-3.236619
6	-7.896131	3.738529	-2.103748
6	-8.084424	-3.795011	1.500439
6	-8.226149	-4.052056	0.063608
6	-8.147326	4.240948	0.713134
6	-8.270506	3.834326	2.076225
6	-8.468992	-3.109963	-2.637478
6	-8.570371	-2.081288	-3.619157
6	-8.574179	1.653132	4.114818
6	-8.726503	0.291847	4.357011
6	-8.799049	0.832263	-4.283732
6	-8.912664	2.128475	-3.799708
6	-9.063514	-2.544403	3.385174
6	-9.212881	-3.428566	2.329105
6	-9.181713	4.077567	-1.514611
6	-9.304528	4.336927	-0.165409
6	-9.517459	-4.027140	-0.608586
6	-9.636631	-3.593726	-1.911186
1	10.629150	3.478235	-2.367961

1	10.422490	4.260458	-0.032549
1	10.297624	-4.482883	0.281324
1	10.084565	-4.022080	-2.136842
1	10.222521	3.740773	2.033704
1	9.958112	2.173853	3.902650
1	9.909848	-2.577707	-3.711083
1	9.710386	-0.287728	-4.563810
1	9.737094	0.112166	4.497311
1	9.469895	-2.286499	4.069254
1	9.574966	1.729465	-3.886164
1	9.283124	-3.688233	2.473323
1	-9.283119	3.688011	2.473685
1	-9.574964	-1.729091	-3.886336
1	-9.469896	2.286102	4.069473
1	-9.737094	-0.112604	4.497301
1	-9.710387	0.288171	-4.563775
1	-9.909850	2.578067	-3.710824
1	-9.958112	-2.174235	3.902440
1	-10.222523	-3.740971	2.033338
1	-10.084564	4.022295	-2.136452
1	-10.297624	4.482859	0.281758
1	-10.422490	-4.260451	-0.032961
1	-10.629150	-3.478001	-2.368296

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B3LYP/STO-3G Energy: -7091.722527

6	-9.719808	-3.091227	-2.704267
6	-9.579104	-3.842719	-1.558454
6	-9.464369	4.128583	1.009538
6	-9.353416	4.226702	-0.361330
6	-9.244986	-4.016232	1.431437
6	-9.093700	-3.430883	2.677186
6	-9.086682	2.933831	-3.072185
6	-8.963233	1.807158	-3.872794
6	-8.781845	-0.932967	4.339676
6	-8.650384	0.446505	4.452730
6	-8.692504	-1.175792	-3.976204
6	-8.566841	-2.419441	-3.292605
6	-8.398766	3.081733	3.038174
6	-8.295957	3.826244	1.825307
6	-8.278650	-4.020170	-0.926515
6	-8.121961	-4.139028	0.525662
6	-8.069900	4.068537	-1.027939
6	-7.946966	3.465132	-2.361169
6	-7.805338	-2.952517	3.125805
6	-7.655989	-1.754731	3.972205
6	-7.691382	1.150009	-4.045048
6	-7.567723	-0.326776	-4.156651
6	-7.383159	1.094748	4.239675
6	-7.266780	2.429455	3.591450
6	-7.257518	-2.873828	-2.890599
6	-7.116225	-3.705417	-1.709629
6	-6.999094	4.015273	1.222815
6	-6.889182	4.162434	-0.216418
6	-6.807479	-4.007283	1.096480
6	-6.650150	-3.431077	2.419475
6	-6.646271	3.052331	-2.819271
6	-6.519724	1.898141	-3.689155
6	-6.350845	-1.170195	4.116526
6	-6.213194	0.263508	4.280196
6	-6.245084	-0.911447	-4.019138
6	-6.094585	-2.217111	-3.434581
6	-5.949958	2.860208	3.151348
6	-5.819947	3.704108	1.994055
6	-5.787598	-3.922608	-1.164553
6	-5.632227	-4.115074	0.246083
6	-5.573301	4.076165	-0.827637

6	-5.451469	3.552790	-2.156009
6	-5.317676	-3.058283	2.873211
6	-5.167580	-1.943328	3.762111
6	-5.193141	1.338442	-3.929523
6	-5.059929	-0.076957	-4.146381
6	-4.885521	0.861449	4.177321
6	-4.757013	2.195642	3.652488
6	-4.769006	-2.707770	-3.088263
6	-4.620239	-3.605068	-1.965559
6	-4.505718	3.953912	1.422361
6	-4.387843	4.183213	-0.001190
6	-4.307408	-4.066654	0.831396
6	-4.151733	-3.567190	2.183920
6	-4.142722	3.213773	-2.671937
6	-4.018127	2.109223	-3.607963
6	-3.852714	-1.398113	4.007620
6	-3.714339	0.027871	4.260401
6	-3.749455	-0.682361	-4.106615
6	-3.605981	-2.039768	-3.607606
6	-3.452399	2.692653	3.286676
6	-3.328059	3.621694	2.176201
6	-3.304808	-3.869012	-1.437322
6	-3.149655	-4.139337	-0.021093
6	-3.086525	4.143207	-0.620651
6	-2.966353	3.684067	-1.989628
6	-2.837879	-3.228581	2.666711
6	-2.688451	-2.151489	3.621681
6	-2.710968	1.563923	-3.884582
6	-2.577341	0.156487	-4.176236
6	-2.404563	0.630972	4.195390
6	-2.272955	1.993603	3.739948
6	-2.289096	-2.540054	-3.278580
6	-2.138563	-3.494239	-2.209285
6	-2.020294	3.885586	1.613131
6	-1.899606	4.188435	0.209525
6	-1.824164	-4.102664	0.567092
6	-1.668066	-3.682336	1.935879
6	-1.652987	3.356111	-2.515269
6	-1.526865	2.314358	-3.503677
6	-1.365448	-1.612283	3.883944
6	-1.224106	-0.216076	4.216617
6	-1.257757	-0.451318	-4.165047
6	-1.115397	-1.828902	-3.753129
6	-0.957645	2.507510	3.398458
6	-0.832787	3.496632	2.350656
6	-0.813751	-3.784296	-1.692317
6	-0.658321	-4.132022	-0.294221
6	-0.589796	4.179433	-0.413220
6	-0.470064	3.795955	-1.807755
6	-0.346794	-3.374816	2.441976
6	-0.197391	-2.351953	3.462425
6	-0.218278	1.788168	-3.821216
6	-0.086563	0.390817	-4.198211
6	0.086563	0.390751	4.198217
6	0.218278	1.788108	3.821245
6	0.197391	-2.351899	-3.462462
6	0.346794	-3.374778	-2.442029
6	0.470064	3.795927	1.807815
6	0.589796	4.179427	0.413287
6	0.658321	-4.132027	0.294156
6	0.813750	-3.784322	1.692257
6	0.832787	3.496668	-2.350600
6	0.957645	2.507563	-3.398418
6	1.115397	-1.828961	3.753100
6	1.257757	-0.451384	4.165040
6	1.224106	-0.216010	-4.216620
6	1.365448	-1.612222	-3.883969
6	1.526865	2.314303	3.503714
6	1.652987	3.356072	2.515323
6	1.668066	-3.682305	-1.935937

6	1.824164	-4.102655	-0.567157
6	1.899606	4.188438	-0.209458
6	2.020294	3.885612	-1.613069
6	2.138563	-3.494273	2.209231
6	2.289095	-2.540106	3.278540
6	2.272955	1.993662	-3.739916
6	2.404564	0.631037	-4.195379
6	2.577341	0.156421	4.176238
6	2.710969	1.563861	3.884606
6	2.688452	-2.151433	-3.621715
6	2.837879	-3.228540	-2.666762
6	2.966353	3.684036	1.989686
6	3.086525	4.143197	0.620717
6	3.149655	-4.139337	0.021028
6	3.304808	-3.869035	1.437262
6	3.328059	3.621728	-2.176143
6	3.452399	2.692704	-3.286633
6	3.605981	-2.039825	3.607575
6	3.749455	-0.682426	4.106605
6	3.714339	0.027938	-4.260400
6	3.852714	-1.398050	-4.007642
6	4.018127	2.109166	3.607995
6	4.142723	3.213730	2.671988
6	4.151733	-3.567156	-2.183975
6	4.307407	-4.066641	-0.831460
6	4.387843	4.183214	0.001256
6	4.505718	3.953936	-1.422299
6	4.620239	-3.605100	1.965503
6	4.769005	-2.707820	3.088221
6	4.757014	2.195699	-3.652453
6	4.885522	0.861514	-4.177308
6	5.059929	-0.077023	4.146380
6	5.193141	1.338379	3.929543
6	5.167580	-1.943269	-3.762141
6	5.317676	-3.058238	-2.873258
6	5.451469	3.552756	2.156064
6	5.573300	4.076153	0.827700
6	5.632226	-4.115071	-0.246147
6	5.787598	-3.922628	1.164492
6	5.819946	3.704141	-1.993997
6	5.949958	2.860258	-3.151302
6	6.094585	-2.217167	3.434547
6	6.245084	-0.911511	4.019123
6	6.213194	0.263575	-4.280192
6	6.350845	-1.170131	-4.116544
6	6.519724	1.898082	3.689182
6	6.646271	3.052285	2.819316
6	6.650150	-3.431039	-2.419528
6	6.807478	-4.007267	-1.096542
6	6.889182	4.162432	0.216482
6	6.999093	4.015296	-1.222753
6	7.116225	-3.705446	1.709572
6	7.257518	-2.873876	2.890555
6	7.266780	2.429511	-3.591410
6	7.383159	1.094815	-4.239655
6	7.567723	-0.326843	4.156646
6	7.691383	1.149944	4.045064
6	7.655989	-1.754669	-3.972232
6	7.805338	-2.952468	-3.125851
6	7.946967	3.465093	2.361221
6	8.069900	4.068523	1.028002
6	8.121960	-4.139021	-0.525727
6	8.278649	-4.020188	0.926452
6	8.295956	3.826278	-1.825248
6	8.398766	3.081785	-3.038127
6	8.566841	-2.419495	3.292566
6	8.692504	-1.175856	3.976184
6	8.650386	0.446575	-4.452718
6	8.781847	-0.932898	-4.339686
6	8.963233	1.807095	3.872819

6	9.086682	2.933782	3.072226
6	9.093700	-3.430843	-2.677240
6	9.244986	-4.016212	-1.431500
6	9.353415	4.226702	0.361395
6	9.464367	4.128608	-1.009475
6	9.579105	-3.842746	1.558394
6	9.719808	-3.091271	2.704217
1	-10.719176	-2.877343	-3.108001
1	-10.473702	-4.230548	-1.054330
1	-10.453944	4.141308	1.487127
1	-10.262094	4.321407	-0.969784
1	-10.253877	-4.259776	1.074628
1	-9.985912	-3.221413	3.281304
1	-10.087793	3.332440	-2.863937
1	-9.870765	1.340399	-4.277170
1	-9.785027	-1.376293	4.381277
1	-9.554384	1.056144	4.579727
1	-9.704256	-0.781184	-4.135414
1	-9.404753	2.822927	3.392929
1	9.404753	2.822988	-3.392887
1	9.704256	-0.781249	4.135395
1	9.554385	1.056217	-4.579704
1	9.785029	-1.376225	-4.381294
1	9.870767	1.340328	4.277183
1	10.087795	3.332388	2.863979
1	9.985912	-3.221363	-3.281354
1	10.253876	-4.259761	-1.074695
1	10.262093	4.321399	0.969850
1	10.453943	4.141342	-1.487064
1	10.473701	-4.230566	1.054262
1	10.719176	-2.877391	3.107954

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B3LYP/STO-3G Energy: -7167.019723

6	-9.811057	-2.206463	-3.492272
6	-9.693447	-3.227591	-2.575917
6	-9.550249	3.811383	1.946173
6	-9.417943	4.256933	0.648508
6	-9.402915	-4.167275	0.273032
6	-9.263954	-3.923618	1.628446
6	-9.120310	3.702586	-2.300312
6	-8.994120	2.818114	-3.361221
6	-8.954863	-1.940307	3.879883
6	-8.814227	-0.637906	4.343839
6	-8.748154	-0.042357	-4.219427
6	-8.643498	-1.419923	-3.875460
6	-8.522487	2.267922	3.651695
6	-8.396138	3.296461	2.671985
6	-8.403204	-3.576898	-1.995238
6	-8.267972	-4.066023	-0.621647
6	-8.125162	4.260704	-0.020466
6	-7.986692	4.019092	-1.461380
6	-7.977317	-3.591046	2.199532
6	-7.829995	-2.652960	3.326034
6	-7.724758	2.210758	-3.679641
6	-7.612472	0.811137	-4.163790
6	-7.538464	0.029413	4.318070
6	-7.402892	1.483634	4.034491
6	-7.343796	-1.978745	-3.588834
6	-7.226873	-3.086947	-2.659042
6	-7.088779	3.620255	2.154923
6	-6.956098	4.130578	0.803037
6	-6.960316	-4.101892	-0.021142
6	-6.816469	-3.886300	1.407366
6	-6.682539	3.722740	-1.994039
6	-6.552405	2.828595	-3.129522
6	-6.522382	-2.139863	3.630679

6	-6.375920	-0.797389	4.158208
6	-6.297698	0.194453	-4.165230
6	-6.167627	-1.219365	-3.933089
6	-6.077149	1.998635	3.736140
6	-5.923978	3.109309	2.835394
6	-5.908536	-3.453131	-2.172931
6	-5.774703	-4.002100	-0.857149
6	-5.632230	4.188748	0.206580
6	-5.494244	4.021430	-1.209399
6	-5.487590	-3.656830	1.956329
6	-5.340676	-2.808807	3.102436
6	-5.227338	2.332078	-3.487635
6	-5.103305	1.019042	-4.058413
6	-5.042310	-0.207659	4.226731
6	-4.896277	1.214256	4.064125
6	-4.851510	-1.798814	-3.708405
6	-4.726885	-2.954907	-2.852672
6	-4.599236	3.482903	2.363162
6	-4.458122	4.067147	1.048266
6	-4.457200	-4.120645	-0.263684
6	-4.315874	-3.985388	1.172246
6	-4.179662	3.809445	-1.778300
6	-4.049807	2.980326	-2.963431
6	-4.024132	-2.359079	3.494090
6	-3.878215	-1.047902	4.106200
6	-3.798158	0.407341	-4.159660
6	-3.674434	-1.034036	-4.025806
6	-3.582478	1.774675	3.855077
6	-3.435154	2.956611	3.022478
6	-3.421062	-3.362778	-2.395476
6	-3.288246	-3.988098	-1.093733
6	-3.147818	4.173179	0.455847
6	-3.010050	4.076785	-0.983704
6	-3.005819	-3.796867	1.740518
6	-2.860856	-3.001210	2.941167
6	-2.743417	2.508123	-3.353959
6	-2.617955	1.220930	-3.996477
6	-2.563425	-0.462871	4.213957
6	-2.415334	0.969831	4.127187
6	-2.367693	-1.618962	-3.822225
6	-2.241395	-2.818024	-3.032598
6	-2.118069	3.342435	2.562827
6	-1.974065	3.992200	1.285083
6	-1.971318	-4.118535	-0.500768
6	-1.830396	-4.062016	0.931252
6	-1.691836	3.876604	-1.558151
6	-1.559097	3.119820	-2.776792
6	-1.537269	-2.561016	3.346701
6	-1.389622	-1.299476	4.028588
6	-1.304412	0.613747	-4.124701
6	-1.180688	-0.823683	-4.082270
6	-1.091251	1.540200	3.945578
6	-0.943914	2.764281	3.191198
6	-0.926478	-3.247507	-2.591978
6	-0.793610	-3.941391	-1.328673
6	-0.654300	4.127731	0.697282
6	-0.515425	4.108300	-0.745710
6	-0.512589	-3.907888	1.513518
6	-0.368794	-3.180829	2.762120
6	-0.248960	2.674715	-3.200417
6	-0.123944	1.421345	-3.922875
6	-0.073646	-0.722762	4.182526
6	0.073646	0.723110	4.182466
6	0.123944	-1.421673	-3.922757
6	0.248960	-2.674984	-3.200195
6	0.368794	3.181060	2.761856
6	0.512588	3.908014	1.513193
6	0.515424	-4.108364	-0.745368
6	0.654300	-4.127674	0.697625
6	0.793609	3.941278	-1.329000

6	0.926477	3.247289	-2.592248
6	0.943915	-2.764015	3.191426
6	1.091251	-1.539871	3.945705
6	1.180688	0.823342	-4.082338
6	1.304413	-0.614092	-4.124650
6	1.389623	1.299812	4.028481
6	1.537269	2.561296	3.346489
6	1.559097	-3.120053	-2.776534
6	1.691835	-3.876736	-1.557829
6	1.830396	4.062094	0.930915
6	1.971318	4.118492	-0.501110
6	1.974065	-3.992094	1.285415
6	2.118070	-3.342221	2.563104
6	2.241395	2.817769	-3.032832
6	2.367694	1.618642	-3.822359
6	2.415335	-0.969487	4.127267
6	2.563426	0.463222	4.213918
6	2.617955	-1.221265	-3.996376
6	2.743417	-2.508404	-3.353751
6	2.860855	3.001456	2.940919
6	3.005818	3.797012	1.740203
6	3.010049	-4.076869	-0.983366
6	3.147818	-4.173142	0.456194
6	3.288246	3.988006	-1.094064
6	3.421061	3.362576	-2.395755
6	3.435155	-2.956359	3.022722
6	3.582479	-1.774354	3.855222
6	3.674434	1.033700	-4.025892
6	3.798158	-0.407689	-4.159626
6	3.878215	1.048245	4.106114
6	4.024132	2.359371	3.493895
6	4.049806	-2.980575	-2.963185
6	4.179661	-3.809595	-1.777984
6	4.315873	3.985486	1.171915
6	4.457199	4.120623	-0.264026
6	4.458122	-4.067061	1.048604
6	4.599238	-3.482706	2.363450
6	4.726885	2.954667	-2.852916
6	4.851510	1.798503	-3.708554
6	4.896278	-1.213917	4.064225
6	5.042311	0.208013	4.226713
6	5.103306	-1.019381	-4.058329
6	5.227338	-2.332371	-3.487442
6	5.340675	2.809068	3.102204
6	5.487588	3.656996	1.956026
6	5.494243	-4.021535	-1.209066
6	5.632230	-4.188733	0.206928
6	5.774702	4.002028	-0.857481
6	5.908535	3.452950	-2.173217
6	5.923979	-3.109071	2.835649
6	6.077151	-1.998321	3.736302
6	6.167628	1.219036	-3.933188
6	6.297699	-0.194802	-4.165212
6	6.375920	0.797739	4.158141
6	6.522382	2.140169	3.630502
6	6.552404	-2.828859	-3.129287
6	6.682537	-3.722911	-1.993731
6	6.816468	3.886421	1.407044
6	6.960314	4.101893	-0.021482
6	6.956098	-4.130513	0.803379
6	7.088780	-3.620074	2.155221
6	7.226873	3.086725	-2.659297
6	7.343797	1.978444	-3.588996
6	7.402894	-1.483293	4.034607
6	7.538465	-0.029050	4.318067
6	7.612473	-0.811486	-4.163717
6	7.724758	-2.211068	-3.679456
6	7.829994	2.653243	3.325815
6	7.977315	3.591236	2.199236
6	7.986691	-4.019219	-1.461048

6	8.125160	-4.260710	-0.020115
6	8.267970	4.065974	-0.621984
6	8.403203	3.576733	-1.995533
6	8.396141	-3.296232	2.672251
6	8.522490	-2.267608	3.651870
6	8.643500	1.419597	-3.875569
6	8.748158	0.042001	-4.219412
6	8.814227	0.638273	4.343782
6	8.954862	1.940636	3.879722
6	8.994119	-2.818399	-3.360987
6	9.120308	-3.702786	-2.300007
6	9.263953	3.923761	1.628122
6	9.402913	4.167304	0.272687
6	9.417943	-4.256881	0.648855
6	9.550251	-3.811214	1.946481
6	9.693447	3.227377	-2.576181
6	9.811058	2.206170	-3.492447
1	-10.802442	-1.884565	-3.840146
1	-10.598330	-3.721452	-2.198874
1	-10.546619	3.712726	2.398972
1	-10.316337	4.515808	0.073398
1	-10.408526	-4.300306	-0.145912
1	-10.162301	-3.867171	2.256674
1	-10.120716	4.048270	-2.010235
1	-9.898738	2.483016	-3.885039
1	-9.961651	-2.369235	3.796248
1	-9.714673	-0.071124	4.613996
1	-9.753689	0.392633	-4.284870
1	-9.535267	1.937764	3.916144
1	9.535275	-1.937413	3.916277
1	9.753700	-0.393000	-4.284793
1	9.714674	0.071513	4.613982
1	9.961650	2.369556	3.796049
1	9.898738	-2.483344	-3.884832
1	10.120713	-4.048450	-2.009904
1	10.162299	3.867368	2.256355
1	10.408523	4.300301	-0.146269
1	10.316336	-4.515805	0.073767
1	10.546623	-3.712515	2.399270
1	10.598329	3.721272	-2.199178
1	10.802443	1.884243	-3.840294

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B3LYP/STO-3G Energy: -7242.316575

6	9.959075	-1.296405	3.839239
6	9.823619	-2.516631	3.216678
6	9.642740	3.123742	-2.955700
6	9.532582	3.887974	-1.814444
6	9.485744	-4.152456	0.707320
6	9.326542	-4.263781	-0.662514
6	9.276565	4.112707	1.181823
6	9.161814	3.531963	2.435424
6	8.989569	-2.924305	-3.344012
6	8.847189	-1.784071	-4.124335
6	8.915871	0.989721	4.001213
6	8.800246	-0.428153	4.023238
6	8.580582	1.204071	-4.194186
6	8.474644	2.449501	-3.509615
6	8.522796	-2.992845	2.761826
6	8.364704	-3.816119	1.562416
6	8.249594	4.074602	-1.151206
6	8.131624	4.212265	0.304091
6	8.031628	-4.079060	-1.281876
6	7.870141	-3.461198	-2.608571
6	7.893766	3.036778	2.915754
6	7.782330	1.809843	3.743845
6	7.574335	-1.121082	-4.251561

6	7.450344	0.357535	-4.348260
6	7.493733	-1.031759	3.907601
6	7.358504	-2.340502	3.294872
6	7.176669	2.907394	-3.075926
6	7.067374	3.748808	-1.898680
6	7.047666	-3.996032	1.009899
6	6.882288	-4.153195	-0.424159
6	6.834011	4.074742	0.912510
6	6.716429	3.502913	2.241334
6	6.559987	-3.033099	-3.016367
6	6.410904	-1.869443	-3.868719
6	6.465498	1.224627	3.921019
6	6.326193	-0.200531	4.061122
6	6.132504	0.943536	-4.174077
6	5.999220	2.249665	-3.586629
6	6.031929	-2.809104	2.937338
6	5.876006	-3.676172	1.808771
6	5.753485	3.970003	-1.319516
6	5.636009	4.172244	0.093457
6	5.546164	-4.061305	-0.994731
6	5.384323	-3.533787	-2.316893
6	5.394676	3.124729	2.731572
6	5.272991	2.003408	3.620799
6	5.079199	-1.304986	-4.065773
6	4.942566	0.111179	-4.271698
6	5.004163	-0.807900	4.009680
6	4.862210	-2.143473	3.482408
6	4.683681	2.743718	-3.207869
6	4.565762	3.646714	-2.086466
6	4.548498	-3.933291	1.284005
6	4.385137	-4.169188	-0.135504
6	4.328375	4.124080	0.715239
6	4.211842	3.626936	2.073693
6	4.062570	-3.187839	-2.791461
6	3.912354	-2.076544	-3.716110
6	3.966094	1.448306	3.892555
6	3.834478	0.022132	4.135444
6	3.634201	0.718250	-4.195485
6	3.506169	2.075933	-3.694350
6	3.547923	-2.646104	3.164453
6	3.393074	-3.584673	2.069458
6	3.264872	3.914296	-1.524027
6	3.148374	4.190735	-0.105875
6	3.067037	-4.123168	-0.714448
6	2.905721	-3.658627	-2.076489
6	2.909217	3.281221	2.589248
6	2.787393	2.201829	3.541438
6	2.598875	-1.527455	-3.951137
6	2.459181	-0.118911	-4.234104
6	2.522892	-0.585373	4.106606
6	2.380410	-1.946751	3.655238
6	2.199081	2.579612	-3.332429
6	2.078396	3.537895	-2.263295
6	2.067433	-3.853810	1.548639
6	1.904337	-4.164091	0.152435
6	1.838415	4.155038	0.518004
6	1.719758	3.734493	1.890182
6	1.577878	-3.324151	-2.560519
6	1.424520	-2.277411	-3.538267
6	1.472978	1.657535	3.836760
6	1.342544	0.259306	4.167121
6	1.141151	0.490947	-4.185440
6	1.012042	1.868557	-3.772974
6	1.057069	-2.465815	3.358376
6	0.902606	-3.461359	2.320382
6	0.768160	3.831895	-1.712127
6	0.650748	4.182454	-0.311934
6	0.577189	-4.153892	-0.431062
6	0.415446	-3.765984	-1.819437
6	0.412851	3.422280	2.429909

6	0.292583	2.395787	3.449319
6	0.107448	-1.746935	-3.813893
6	-0.032835	-0.349834	-4.184687
6	0.032835	-0.349702	4.184699
6	-0.107448	-1.746815	3.813947
6	-0.292583	2.395678	-3.449393
6	-0.412851	3.422203	-2.430015
6	-0.415446	-3.765927	1.819556
6	-0.577188	-4.153879	0.431193
6	-0.650748	4.182464	0.311804
6	-0.768160	3.831949	1.712008
6	-0.902606	-3.461433	-2.320273
6	-1.057069	-2.465921	-3.358298
6	-1.012042	1.868676	3.772916
6	-1.141151	0.491079	4.185425
6	-1.342545	0.259175	-4.167128
6	-1.472978	1.657415	-3.836811
6	-1.424520	-2.277300	3.538338
6	-1.577878	-3.324071	2.560623
6	-1.719758	3.734433	-1.890298
6	-1.838415	4.155022	-0.518134
6	-1.904337	-4.164097	-0.152304
6	-2.067433	-3.853860	-1.548518
6	-2.078396	3.537966	2.263186
6	-2.199082	2.579717	3.332349
6	-2.380410	-1.946866	-3.655176
6	-2.522892	-0.585502	-4.106586
6	-2.459182	-0.118778	4.234107
6	-2.598875	-1.527331	3.951184
6	-2.787393	2.201717	-3.541506
6	-2.909217	3.281139	-2.589349
6	-2.905721	-3.658562	2.076604
6	-3.067037	-4.123147	0.714577
6	-3.148374	4.190739	0.105745
6	-3.264872	3.914345	1.523905
6	-3.393074	-3.584740	-2.069346
6	-3.547922	-2.646205	-3.164370
6	-3.506169	2.076050	3.694285
6	-3.634202	0.718382	4.195463
6	-3.834478	0.022002	-4.135443
6	-3.966094	1.448183	-3.892598
6	-3.912354	-2.076427	3.716174
6	-4.062571	-3.187751	2.791560
6	-4.211842	3.626871	-2.073805
6	-4.328375	4.124058	-0.715367
6	-4.385137	-4.169185	0.135634
6	-4.548497	-3.933333	-1.283882
6	-4.565762	3.646780	2.086352
6	-4.683682	2.743819	3.207784
6	-4.862210	-2.143584	-3.482341
6	-5.004163	-0.808026	-4.009653
6	-4.942567	0.111313	4.271694
6	-5.079199	-1.304858	4.065812
6	-5.272991	2.003294	-3.620860
6	-5.394676	3.124643	-2.731668
6	-5.384323	-3.533714	2.317002
6	-5.546164	-4.061275	0.994857
6	-5.636009	4.172242	-0.093587
6	-5.753485	3.970046	1.319392
6	-5.876005	-3.676231	-1.808657
6	-6.031929	-2.809198	-2.937250
6	-5.999221	2.249778	3.586559
6	-6.132504	0.943668	4.174046
6	-6.326193	-0.200659	-4.061114
6	-6.465498	1.224503	-3.921055
6	-6.410905	-1.869320	3.868775
6	-6.559988	-3.033004	3.016459
6	-6.716429	3.502843	-2.241442
6	-6.834011	4.074715	-0.912637
6	-6.882288	-4.153183	0.424288

6	-7.047665	-3.996066	-1.009775
6	-7.067374	3.748869	1.898563
6	-7.176670	2.907491	3.075834
6	-7.358504	-2.340607	-3.294799
6	-7.493733	-1.031883	-3.907568
6	-7.450345	0.357672	4.348247
6	-7.574336	-1.120948	4.251593
6	-7.782330	1.809725	-3.743900
6	-7.893766	3.036687	-2.915849
6	-7.870141	-3.461117	2.608677
6	-8.031628	-4.079022	1.282002
6	-8.131624	4.212257	-0.304223
6	-8.249594	4.074640	1.151079
6	-8.364704	-3.816170	-1.562298
6	-8.522796	-2.992934	-2.761733
6	-8.474645	2.449612	3.509538
6	-8.580582	1.204203	4.194147
6	-8.800246	-0.428280	-4.023225
6	-8.915870	0.989594	-4.001246
6	-8.847189	-1.783942	4.124389
6	-8.989569	-2.924202	3.344103
6	-9.161814	3.531889	-2.435535
6	-9.276565	4.112673	-1.181952
6	-9.326542	-4.263762	0.662646
6	-9.485744	-4.152480	-0.707191
6	-9.532582	3.888035	1.814323
6	-9.642740	3.123839	2.955604
6	-9.823618	-2.516734	-3.216601
6	-9.959075	-1.296527	-3.839199
1	10.956668	-0.904126	4.080905
1	10.720422	-3.098436	2.967444
1	10.631348	2.903898	-3.382024
1	10.440695	4.278543	-1.337309
1	10.497062	-4.181990	1.132502
1	10.214824	-4.378443	-1.297076
1	10.273941	4.365294	0.799809
1	10.072072	3.336432	3.016975
1	9.995339	-3.327264	-3.168824
1	9.745144	-1.313869	-4.545762
1	9.923978	1.419529	3.939840
1	9.587194	0.807893	-4.379528
1	-9.587193	0.808032	4.379503
1	-9.923974	1.419404	-3.939897
1	-9.745144	-1.313727	4.545802
1	-9.995337	-3.327169	3.168933
1	-10.072072	3.336340	-3.017080
1	-10.273940	4.365273	-0.799947
1	-10.214824	-4.378403	1.297211
1	-10.497062	-4.182025	-1.132372
1	-10.440694	4.278591	1.337177
1	-10.631347	2.904012	3.381936
1	-10.720422	-3.098532	-2.967350
1	-10.956667	-0.904256	-4.080877

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6	-10.000252	-0.239162	-4.162487
6	-9.875378	-1.578068	-3.870198
6	-9.793120	2.290784	3.547050
6	-9.665545	3.320227	2.640770
6	-9.579606	-3.800761	-1.855062
6	-9.442633	-4.259072	-0.557388
6	-9.362517	4.302207	-0.194854
6	-9.227272	4.062150	-1.552944
6	-9.146962	-3.654727	2.383411
6	-9.015975	-2.754288	3.432087
6	-8.954455	2.007251	-3.715538

6	-8.838213	0.642811	-4.098118
6	-8.749722	0.114476	4.268946
6	-8.633226	1.492249	3.927431
6	-8.582004	-2.160240	-3.529997
6	-8.444146	-3.262282	-2.578798
6	-8.371927	3.665127	2.066141
6	-8.231204	4.169733	0.697328
6	-8.157057	-4.245551	0.108677
6	-8.016051	-3.989679	1.550871
6	-7.950561	3.702464	-2.124594
6	-7.824825	2.729503	-3.237531
6	-7.744234	-2.151376	3.743922
6	-7.621312	-0.748172	4.218022
6	-7.533390	0.023980	-4.119975
6	-7.408591	-1.398496	-3.860609
6	-7.328480	2.041155	3.645198
6	-7.201294	3.155417	2.724115
6	-7.136163	-3.584629	-2.070696
6	-6.994134	-4.104414	-0.722092
6	-6.923957	4.189442	0.094193
6	-6.784694	3.976844	-1.335090
6	-6.712100	-3.687438	2.074996
6	-6.575536	-2.781821	3.199642
6	-6.505459	2.204066	-3.538008
6	-6.363643	0.861603	-4.036423
6	-6.301322	-0.142287	4.219305
6	-6.159170	1.270246	3.987867
6	-6.088643	-1.948814	-3.613782
6	-5.951860	-3.076649	-2.742681
6	-5.879005	3.512842	2.241048
6	-5.739574	4.069706	0.929322
6	-5.667631	-4.168290	-0.126657
6	-5.526292	-3.997425	1.288337
6	-5.455237	3.731423	-1.884864
6	-5.318248	2.874717	-3.028427
6	-5.246892	-2.291644	3.553611
6	-5.112843	-0.976718	4.116777
6	-5.042449	0.255445	-4.119745
6	-4.909514	-1.170243	-3.950493
6	-4.837665	1.839629	3.767367
6	-4.702746	2.999125	2.917790
6	-4.632851	-3.465932	-2.280452
6	-4.492684	-4.058221	-0.967587
6	-4.421621	4.178243	0.336184
6	-4.282844	4.044967	-1.101337
6	-4.211200	-3.790426	1.855644
6	-4.074438	-2.953404	3.034926
6	-4.006009	2.402092	-3.412076
6	-3.869977	1.085447	-4.009279
6	-3.802689	-0.375540	4.217710
6	-3.667131	1.064684	4.083837
6	-3.600254	-1.743907	-3.751566
6	-3.464154	-2.933354	-2.932862
6	-3.393308	3.398498	2.463520
6	-3.254943	4.029756	1.165679
6	-3.183791	-4.169956	-0.376238
6	-3.043720	-4.069700	1.061862
6	-2.972112	3.838808	-1.667845
6	-2.833766	3.036860	-2.861884
6	-2.764616	-2.488342	3.421965
6	-2.628798	-1.199065	4.057557
6	-2.559305	0.485321	-4.115287
6	-2.424792	-0.947389	-4.026674
6	-2.355139	1.639434	3.882755
6	-2.218579	2.840379	3.098614
6	-2.148082	-3.334401	-2.478601
6	-2.008095	-3.993866	-1.206711
6	-1.935989	4.151318	0.573908
6	-1.795061	4.094824	-0.857448
6	-1.723839	-3.875609	1.634953

6	-1.584681	-3.112858	2.848233
6	-1.514508	2.579580	-3.263428
6	-1.378031	1.311927	-3.935963
6	-1.309764	-0.602126	4.184441
6	-1.174273	0.833919	4.141805
6	-1.106732	-1.531394	-3.850746
6	-0.970133	-2.761086	-3.104391
6	-0.899721	3.262145	2.661573
6	-0.760813	3.961608	1.402172
6	-0.690029	-4.140435	-0.619634
6	-0.549800	-4.120246	0.822487
6	-0.478506	3.926572	-1.438477
6	-0.340079	3.191673	-2.681333
6	-0.270700	-2.675394	3.268788
6	-0.135472	-1.419680	3.985080
6	-0.066827	0.721557	-4.085692
6	0.066827	-0.723750	-4.085305
6	0.135473	1.421821	3.984319
6	0.270700	2.677150	3.267354
6	0.340079	-3.193113	-2.679623
6	0.478505	-3.927344	-1.436372
6	0.549799	4.120690	0.820278
6	0.690028	4.140102	-0.621854
6	0.760813	-3.960853	1.404295
6	0.899721	-3.260713	2.663321
6	0.970133	2.759418	-3.105869
6	1.106733	1.529326	-3.851565
6	1.174275	-0.831694	4.142250
6	1.309765	0.604373	4.184117
6	1.378031	-1.314040	-3.935259
6	1.514508	-2.581333	-3.262046
6	1.584680	3.114390	2.846565
6	1.723838	3.876489	1.632875
6	1.795059	-4.095285	-0.855253
6	1.935988	-4.151008	0.576133
6	2.008095	3.993218	-1.208852
6	2.148082	3.333069	-2.480386
6	2.218579	-2.838713	3.100134
6	2.355140	-1.637348	3.883630
6	2.424793	0.945226	-4.027179
6	2.559305	-0.487531	-4.115026
6	2.628799	1.201246	4.056913
6	2.764616	2.490182	3.420631
6	2.833765	-3.038399	-2.860257
6	2.972110	-3.839706	-1.665788
6	3.043718	4.070273	1.059680
6	3.183791	4.169755	-0.378473
6	3.254943	-4.029129	1.167838
6	3.393309	-3.397173	2.465339
6	3.464155	2.931776	-2.934431
6	3.600255	1.741891	-3.752497
6	3.667132	-1.062488	4.084403
6	3.802690	0.377807	4.217506
6	3.869977	-1.087602	-4.008697
6	4.006007	-2.403927	-3.410791
6	4.074437	2.955038	3.033344
6	4.211198	3.791427	1.853614
6	4.282842	-4.045562	-1.099170
6	4.421620	-4.178064	0.338422
6	4.492684	4.057702	-0.969761
6	4.632852	3.464705	-2.282307
6	4.702747	-2.997555	2.919392
6	4.837667	-1.837602	3.768347
6	4.909516	1.168119	-3.951115
6	5.042450	-0.257660	-4.119607
6	5.112844	0.978931	4.116251
6	5.246891	2.293557	3.552384
6	5.318246	-2.876349	-3.026890
6	5.455234	-3.732442	-1.882867
6	5.526291	3.998122	1.286196

6	5.667631	4.168225	-0.128890
6	5.739573	-4.069207	0.931501
6	5.879006	-3.511635	2.242925
6	5.951862	3.075171	-2.744324
6	6.088645	1.946868	-3.614819
6	6.159172	-1.268101	3.988539
6	6.301323	0.144556	4.219223
6	6.363643	-0.863776	-4.035961
6	6.505457	-2.205973	-3.536831
6	6.575534	2.783547	3.198154
6	6.712098	3.688561	2.073023
6	6.784691	-3.977568	-1.332962
6	6.923955	-4.189395	0.096435
6	6.994134	4.104027	-0.724289
6	7.136165	3.583512	-2.072611
6	7.201296	-3.153948	2.725797
6	7.328483	-2.039191	3.646282
6	7.408592	1.396415	-3.861350
6	7.533391	-0.026198	-4.119958
6	7.621313	0.750443	4.217618
6	7.744233	2.153395	3.742773
6	7.824823	-2.731251	-3.236073
6	7.950558	-3.703616	-2.122615
6	8.016050	3.990522	1.548738
6	8.157057	4.245614	0.106405
6	8.231203	-4.169361	0.699557
6	8.371928	-3.664013	2.068096
6	8.444148	3.260888	-2.580537
6	8.582007	2.158334	-3.531143
6	8.633228	-1.490133	3.928218
6	8.749723	-0.112178	4.269002
6	8.838213	-0.645019	-4.097770
6	8.954455	-2.009254	-3.714460
6	9.015973	2.756144	3.430619
6	9.146960	3.656022	2.381461
6	9.227269	-4.062995	-1.550774
6	9.362515	-4.302319	-0.192555
6	9.442633	4.258773	-0.559664
6	9.579608	3.799756	-1.857089
6	9.665546	-3.318800	2.642536
6	9.793122	-2.288870	3.548262
6	9.875380	1.575978	-3.871030
6	10.000253	0.236917	-4.162606
1	-10.993402	0.206154	-4.313585
1	-10.775956	-2.200987	-3.793941
1	-10.787980	1.973541	3.889231
1	-10.565984	3.824084	2.266298
1	-10.583764	-3.716266	-2.289736
1	-10.340857	-4.528593	0.013073
1	-10.365838	4.452546	0.223751
1	-10.127623	4.026351	-2.179905
1	-10.149884	-3.995762	2.096202
1	-9.919670	-2.404891	3.948097
1	-9.963276	2.411806	-3.563234
1	-9.759014	-0.312228	4.332281
1	9.759012	0.314558	4.332114
1	9.963283	-2.413723	-3.561923
1	9.919668	2.407026	3.946818
1	10.149880	3.996905	2.094070
1	10.127619	-4.027533	-2.177755
1	10.365836	-4.452432	0.226130
1	10.340857	4.528602	0.010651
1	10.583768	3.715022	-2.291716
1	10.565986	-3.822857	2.268333
1	10.787983	-1.971442	3.890270
1	10.775959	2.198937	-3.795102
1	10.993404	-0.208480	-4.313464

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B3LYP/STO-3G Energy: -7392.909326

6	-10.165641	-3.971577	-0.840383
6	-10.041321	-4.036169	0.528193
6	-9.835351	4.130745	-1.300275
6	-9.717652	3.518075	-2.527891
6	-9.725702	-2.664545	3.193948
6	-9.572262	-1.530746	3.970051
6	-9.454342	1.024943	-4.205055
6	-9.340296	-0.350637	-4.322488
6	-9.231786	1.462156	4.142371
6	-9.081388	2.704855	3.543096
6	-9.105916	-2.974234	-2.894991
6	-8.999532	-3.697341	-1.676380
6	-8.789861	4.249649	0.988295
6	-8.672727	4.273140	-0.430001
6	-8.744961	-3.875062	1.178233
6	-8.597945	-3.242113	2.487064
6	-8.431276	3.030157	-3.008859
6	-8.309686	1.835958	-3.848031
6	-8.276685	-0.902380	4.128542
6	-8.114001	0.553927	4.252475
6	-8.072824	-1.015354	-4.123063
6	-7.966485	-2.342538	-3.470430
6	-7.801701	3.142407	3.041838
6	-7.665307	3.960081	1.809207
6	-7.696886	-3.897420	-1.084484
6	-7.573326	-4.015556	0.356649
6	-7.369815	4.121444	-1.033257
6	-7.252405	3.516812	-2.347289
6	-7.284020	-2.853819	2.930027
6	-7.125111	-1.686649	3.779797
6	-7.011480	1.238334	-4.024066
6	-6.894478	-0.199675	-4.186903
6	-6.801269	1.118743	4.097479
6	-6.644167	2.436785	3.512172
6	-6.653665	-2.788496	-3.041368
6	-6.523419	-3.618022	-1.872497
6	-6.343265	4.097011	1.224385
6	-6.198714	4.235067	-0.200261
6	-6.252326	-3.937723	0.951715
6	-6.107602	-3.388991	2.265927
6	-5.936679	3.121439	-2.817362
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6	-5.790910	-1.147545	3.995431
6	-5.628713	0.260955	4.194988
6	-5.574523	-0.814328	-4.092201
6	-5.457023	-2.141046	-3.558730
6	-5.308495	2.884249	3.129672
6	-5.159965	3.763557	2.004355
6	-5.205455	-3.873175	-1.308235
6	-5.074834	-4.078481	0.112058
6	-4.878175	4.146614	-0.807166
6	-4.751742	3.623498	-2.145754
6	-4.783169	-3.061643	2.761169
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6	-4.505776	1.430266	-3.952499
6	-4.389052	0.006155	-4.194632
6	-4.304009	0.842777	4.142308
6	-4.146138	2.194624	3.637204
6	-4.151476	-2.653267	-3.201482
6	-4.028142	-3.570052	-2.082825
6	-3.845001	3.994965	1.449384
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6	-3.764418	-4.053083	0.717485
6	-3.621352	-3.571501	2.078165
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6	-3.326828	2.175684	-3.595990
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6	-3.149554	-0.013742	4.209979
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6	-1.821402	0.570237	4.171514
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6	-0.659418	-0.296058	4.199997
6	-0.590830	-0.409025	-4.172592
6	-0.472877	-1.799377	-3.781481
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6	-0.185674	3.443400	2.401175
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6	0.338155	-2.441288	3.427608
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6	0.659420	0.287604	4.200583
6	0.820026	1.683025	3.848128
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6	0.951771	-3.376872	-2.473988
6	1.128975	3.723544	1.873966
6	1.271559	4.127051	0.494691
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6	1.898415	-0.207778	-4.184229
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6	2.146078	2.193254	3.554327
6	2.300977	3.250133	2.589597
6	2.265420	-3.713084	-1.954018
6	2.394446	-4.164932	-0.591665
6	2.590357	4.130322	-0.114642
6	2.721325	3.848862	-1.522838
6	2.677526	-3.615412	2.197538
6	2.829010	-2.675103	3.283317
6	2.969530	1.984211	-3.671512
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6	3.149556	0.005269	4.209991
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6	3.326830	-2.168445	-3.600348
6	3.447390	-3.262211	-2.656331
6	3.621350	3.567314	2.085339
6	3.764414	4.051638	0.725632
6	3.705241	-4.233810	0.015150
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6	4.146139	-2.201942	3.632782
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6	4.878173	-4.144991	-0.815499
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6	8.431276	-3.024103	-3.014936
6	8.597943	3.237108	2.493570
6	8.744957	3.872702	1.186020
6	8.672725	-4.272280	-0.438591
6	8.789862	-4.251634	0.979748
6	8.999530	3.700727	-1.668941
6	9.105917	2.980061	-2.888996
6	9.081389	-2.711982	3.537642
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1	10.240090	-1.120930	4.395765
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1	10.463076	1.027007	4.379992
1	10.735369	3.042959	3.007064
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6	2.340984	-3.798306	-1.663129
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6	3.807689	-4.116732	0.337873
6	3.864304	4.067451	-1.110247
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6	4.100424	-2.940748	2.921593
6	4.244563	-1.771334	3.768430
6	4.253966	1.168789	-4.085312
6	4.389675	-0.268489	-4.228169
6	4.523375	1.049972	4.047207
6	4.656282	2.362003	3.448189
6	4.677019	-2.851877	-3.059510
6	4.824496	-3.695571	-1.895484
6	4.917652	4.016359	1.139396
6	5.042073	4.178345	-0.287904
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6	5.268000	-3.448409	2.243938
6	5.300310	3.086727	-2.909572
6	5.429589	1.948098	-3.773448
6	5.559836	-1.203220	3.976793
6	5.698240	0.213171	4.153239
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6	7.620139	-4.047054	0.661533
6	7.756798	-3.565646	2.023650
6	7.808959	3.289567	-2.778445
6	7.926257	2.182427	-3.760804
6	8.065290	-1.456480	3.931484
6	8.193546	-0.009166	4.223438
6	8.194705	-0.633846	-4.272098
6	8.337791	-2.012109	-3.782265
6	8.464699	2.674301	3.229967
6	8.595537	3.612530	2.114177
6	8.638853	-3.860196	-1.599413
6	8.787383	-4.138987	-0.173752
6	8.835653	4.151133	-0.697555
6	8.943234	3.763694	-2.062076
6	9.066995	-3.239400	2.538926
6	9.192592	-2.230824	3.530847
6	9.197076	1.611917	-4.137279
6	9.326214	0.255904	-4.400317
6	9.471488	0.666571	4.242037

6	9.602059	1.964678	3.778076
6	9.626014	-2.600247	-3.474366
6	9.769408	-3.500683	-2.435804
6	9.885087	3.944585	1.520429
6	10.002368	4.221171	0.176999
6	10.086904	-4.148407	0.490932
6	10.222920	-3.736986	1.796213
1	-11.219552	-3.650163	-2.250955
1	-10.981898	-4.395577	0.094399
1	-10.993327	4.365373	0.275569
1	-10.789612	3.873421	-2.138091
1	-10.774711	-3.840511	2.155767
1	-10.520174	-2.240775	3.999708
1	-10.604021	2.404784	-3.694591
1	-10.373828	0.104650	-4.515635
1	-10.327687	-0.163332	4.561683
1	-10.100573	2.233892	4.096612
1	-10.203660	-1.898452	-3.799113
1	-9.949508	3.609082	2.472246
1	9.949505	3.609160	-2.472128
1	10.203657	-1.898579	3.799055
1	10.100572	2.234028	-4.096544
1	10.327685	-0.163180	-4.561692
1	10.373826	0.104500	4.515644
1	10.604020	2.404660	3.694673
1	10.520173	-2.240640	-3.999783
1	10.774711	-3.840434	-2.155893
1	10.789612	3.873342	2.138218
1	10.993328	4.365371	-0.275426
1	10.981899	-4.395564	-0.094545
1	11.219552	-3.650231	2.250834

Nanotube (7,5) u08v04
B3LYP/STO-3G Energy: -7543.500939

6	-10.348107	-3.054145	-2.748298
6	-10.229245	-3.788218	-1.591707
6	-10.061287	4.218913	0.854968
6	-9.932261	4.295068	-0.513077
6	-9.933796	-3.918138	1.405348
6	-9.791527	-3.316193	2.640697
6	-9.645986	2.956867	-3.200589
6	-9.524517	1.819574	-3.980196
6	-9.472828	-0.796208	4.268977
6	-9.327788	0.579730	4.362603
6	-9.284458	-1.166781	-4.031197
6	-9.179507	-2.396768	-3.330522
6	-9.031009	3.187895	2.909207
6	-8.904666	3.910763	1.691540
6	-8.935936	-3.965820	-0.937613
6	-8.798418	-4.064122	0.511858
6	-8.639490	4.109056	-1.162312
6	-8.506563	3.487174	-2.479504
6	-8.500073	-2.841638	3.097787
6	-8.348309	-1.637494	3.925001
6	-8.253680	1.144482	-4.125331
6	-8.144215	-0.330031	-4.212782
6	-8.046928	1.212312	4.154115
6	-7.908501	2.531962	3.489560
6	-7.877670	-2.861646	-2.907635
6	-7.759408	-3.677982	-1.713895
6	-7.596356	4.081201	1.103175
6	-7.466943	4.207039	-0.336713
6	-7.488491	-3.942172	1.098582
6	-7.341246	-3.347847	2.415907
6	-7.203946	3.057598	-2.918884
6	-7.079048	1.888137	-3.770872
6	-7.038576	-1.065993	4.081685

6	-6.887543	0.370039	4.226112
6	-6.831851	-0.927648	-4.053695
6	-6.702721	-2.226939	-3.447140
6	-6.584548	2.944957	3.061528
6	-6.431749	3.770299	1.892736
6	-6.442116	-3.901013	-1.149389
6	-6.306266	-4.073561	0.265203
6	-6.146819	4.097412	-0.930044
6	-6.014221	3.553252	-2.247318
6	-6.012422	-2.980500	2.879239
6	-5.861178	-1.855368	3.750707
6	-5.757260	1.309101	-3.982442
6	-5.636176	-0.106345	-4.174569
6	-5.553349	0.952204	4.125912
6	-5.403951	2.271873	3.584346
6	-5.386057	-2.724457	-3.073802
6	-5.259861	-3.603207	-1.940913
6	-5.106661	3.995089	1.331790
6	-4.968098	4.201662	-0.087464
6	-4.985274	-4.027281	0.866844
6	-4.840448	-3.512033	2.208286
6	-4.699041	3.190290	-2.741074
6	-4.573926	2.075303	-3.655402
6	-4.539070	-1.318963	4.003440
6	-4.387931	0.104143	4.236193
6	-4.328897	-0.726307	-4.110159
6	-4.205993	-2.075089	-3.591535
6	-4.086035	2.752055	3.228401
6	-3.938496	3.663381	2.108494
6	-3.951031	-3.876757	-1.393144
6	-3.816197	-4.129063	0.028426
6	-3.657506	4.143550	-0.690978
6	-3.525176	3.663237	-2.052603
6	-3.527879	-3.183999	2.705423
6	-3.378594	-2.093107	3.647516
6	-3.269912	1.513792	-3.911598
6	-3.148200	0.098383	-4.181348
6	-3.072667	0.693001	4.182097
6	-2.921379	2.049592	3.707727
6	-2.900914	-2.585813	-3.241131
6	-2.773803	-3.526853	-2.154908
6	-2.624241	3.907353	1.558810
6	-2.483215	4.188423	0.151842
6	-2.500660	-4.097733	0.632344
6	-2.357063	-3.658676	1.995845
6	-2.212031	3.311859	-2.555403
6	-2.084827	2.255058	-3.523673
6	-2.055472	-1.562279	3.914664
6	-1.902910	-0.166342	4.225594
6	-1.837116	-0.523154	-4.139884
6	-1.714094	-1.890359	-3.707270
6	-1.597135	2.542360	3.370321
6	-1.448628	3.511188	2.315520
6	-1.457475	-3.818930	-1.614173
6	-1.322149	-4.147151	-0.216645
6	-1.163603	4.152324	-0.455122
6	-1.029363	3.748951	-1.834614
6	-1.034961	-3.354669	2.513178
6	-0.885983	-2.323544	3.515588
6	-0.773613	1.707845	-3.815213
6	-0.651569	0.310346	-4.169668
6	-0.580760	0.427388	4.213398
6	-0.429135	1.813604	3.820072
6	-0.405516	-2.424896	-3.393268
6	-0.279125	-3.432757	-2.359341
6	-0.131904	3.793735	1.785853
6	0.009424	4.157948	0.388935
6	-0.009424	-4.157950	0.388917
6	0.131904	-3.793744	1.785836
6	0.279125	3.432769	-2.359327

6	0.405516	2.424913	-3.393257
6	0.429135	-1.813624	3.820065
6	0.580759	-0.427409	4.213396
6	0.651569	-0.310326	-4.169669
6	0.773613	-1.707826	-3.815220
6	0.885983	2.323527	3.515598
6	1.034961	3.354656	2.513192
6	1.029363	-3.748942	-1.834630
6	1.163603	-4.152322	-0.455140
6	1.322149	4.147152	-0.216627
6	1.457475	3.818938	-1.614156
6	1.448628	-3.511200	2.315505
6	1.597135	-2.542377	3.370311
6	1.714094	1.890377	-3.707262
6	1.837116	0.523174	-4.139881
6	1.902910	0.166322	4.225595
6	2.055472	1.562260	3.914671
6	2.084827	-2.255041	-3.523682
6	2.212032	-3.311846	-2.555417
6	2.357062	3.658666	1.995862
6	2.500660	4.097730	0.632363
6	2.483215	-4.188424	0.151823
6	2.624241	-3.907361	1.558793
6	2.773804	3.526864	-2.154892
6	2.900915	2.585829	-3.241119
6	2.921379	-2.049611	3.707718
6	3.072667	-0.693022	4.182094
6	3.148200	-0.098363	-4.181347
6	3.269912	-1.513773	-3.911603
6	3.378594	2.093089	3.647525
6	3.527879	3.183986	2.705438
6	3.525176	-3.663227	-2.052618
6	3.657506	-4.143547	-0.690996
6	3.816197	4.129063	0.028445
6	3.951032	3.876764	-1.393125
6	3.938496	-3.663391	2.108477
6	4.086035	-2.752071	3.228389
6	4.205993	2.075106	-3.591525
6	4.328897	0.726327	-4.110155
6	4.387931	-0.104163	4.236193
6	4.539070	1.318944	4.003447
6	4.573926	-2.075285	-3.655410
6	4.699041	-3.190277	-2.741088
6	4.840447	3.512022	2.208302
6	4.985274	4.027276	0.866863
6	4.968099	-4.201661	-0.087483
6	5.106662	-3.995096	1.331772
6	5.259861	3.603216	-1.940895
6	5.386057	2.724472	-3.073789
6	5.403951	-2.271891	3.584336
6	5.553349	-0.952223	4.125908
6	5.636176	0.106365	-4.174568
6	5.757260	-1.309081	-3.982448
6	5.861177	1.855350	3.750717
6	6.012422	2.980486	2.879254
6	6.014221	-3.553242	-2.247334
6	6.146819	-4.097408	-0.930063
6	6.306266	4.073560	0.265223
6	6.442116	3.901018	-1.149370
6	6.431750	-3.770308	1.892719
6	6.584548	-2.944972	3.061515
6	6.702721	2.226956	-3.447129
6	6.831851	0.927668	-4.053692
6	6.887543	-0.370059	4.226111
6	7.038575	1.065974	4.081691
6	7.079048	-1.888119	-3.770881
6	7.203946	-3.057585	-2.918899
6	7.341245	3.347836	2.415925
6	7.488490	3.942167	1.098601
6	7.466943	-4.207037	-0.336732

6	7.596357	-4.081205	1.103156
6	7.759408	3.677990	-1.713877
6	7.877670	2.861660	-2.907622
6	7.908501	-2.531979	3.489549
6	8.046928	-1.212332	4.154109
6	8.144214	0.330052	-4.212785
6	8.253680	-1.144462	-4.125339
6	8.348308	1.637477	3.925011
6	8.500072	2.841624	3.097802
6	8.506563	-3.487164	-2.479522
6	8.639490	-4.109050	-1.162333
6	8.798418	4.064119	0.511879
6	8.935936	3.965824	-0.937593
6	8.904666	-3.910770	1.691522
6	9.031009	-3.187908	2.909192
6	9.179506	2.396786	-3.330514
6	9.284457	1.166803	-4.031197
6	9.327788	-0.579750	4.362602
6	9.472827	0.796189	4.268983
6	9.524517	-1.819559	-3.980210
6	9.645986	-2.956856	-3.200608
6	9.791527	3.316182	2.640715
6	9.933796	3.918132	1.405368
6	9.932261	-4.295064	-0.513099
6	10.061288	-4.218914	0.854947
6	10.229245	3.788224	-1.591687
6	10.348107	3.054158	-2.748284
1	-11.339136	-2.841589	-3.172761
1	-11.132322	-4.166738	-1.095654
1	-11.055378	4.255978	1.321786
1	-10.830435	4.397782	-1.135676
1	-10.939464	-4.163748	1.040990
1	-10.686786	-3.093587	3.235550
1	-10.643711	3.374971	-3.015648
1	-10.429545	1.358583	-4.396628
1	-10.479706	-1.230937	4.311428
1	-10.224314	1.202758	4.476909
1	-10.288950	-0.763705	-4.212736
1	-10.042970	2.946075	3.258470
1	10.042975	-2.946085	3.258456
1	10.288959	0.763721	-4.212728
1	10.224314	-1.202778	4.476905
1	10.479705	1.230918	4.311441
1	10.429544	-1.358570	-4.396645
1	10.643708	-3.374964	-3.015673
1	10.686785	3.093573	3.235568
1	10.939463	4.163744	1.041012
1	10.830435	-4.397778	-1.135699
1	11.055379	-4.255980	1.321765
1	11.132322	4.166743	-1.095633
1	11.339136	2.841605	-3.172748

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B3LYP/STO-3G Energy: -7618.796310

6	10.463433	-2.324791	3.361820
6	10.325326	-3.329266	2.433512
6	10.187699	3.780042	-1.978571
6	10.075131	4.206583	-0.675302
6	9.991651	-4.222490	-0.426637
6	9.838210	-3.956967	-1.773249
6	9.809724	3.607648	2.268597
6	9.688877	2.709903	3.314603
6	9.518364	-1.935987	-3.990015
6	9.383091	-0.628792	-4.431122
6	9.428415	-0.161571	4.129005
6	9.306423	-1.527996	3.767676
6	9.125082	2.267221	-3.689478

6	9.018840	3.278979	-2.697353
6	9.022504	-3.655724	1.859505
6	8.866231	-4.121466	0.486400
6	8.788244	4.206825	0.012169
6	8.665642	3.945956	1.445253
6	8.544218	-3.601534	-2.323684
6	8.391244	-2.648926	-3.429894
6	8.414431	2.106526	3.639193
6	8.295561	0.705454	4.101964
6	8.109450	0.050181	-4.378336
6	7.989845	1.496643	-4.072581
6	7.995957	-2.073236	3.491570
6	7.857430	-3.167164	2.548595
6	7.718574	3.609384	-2.160628
6	7.606785	4.102213	-0.800415
6	7.549719	-4.141742	-0.098717
6	7.390113	-3.904158	-1.522988
6	7.364833	3.657132	1.992508
6	7.241096	2.746508	3.117240
6	7.083964	-2.122851	-3.715043
6	6.942546	-0.770058	-4.221333
6	6.977537	0.099976	4.114558
6	6.832264	-1.310263	3.862520
6	6.674761	2.020280	-3.752963
6	6.542550	3.119480	-2.833437
6	6.532177	-3.514868	2.073933
6	6.377483	-4.042988	0.752349
6	6.293163	4.162518	-0.186636
6	6.171457	3.975573	1.227223
6	6.058669	-3.653534	-2.051293
6	5.904941	-2.787801	-3.180304
6	5.917969	2.253631	3.481816
6	5.789064	0.936537	4.031428
6	5.614668	-0.167188	-4.260063
6	5.482614	1.248265	-4.074101
6	5.507832	-1.873896	3.642174
6	5.361814	-3.011966	2.774638
6	5.226090	3.494875	-2.336543
6	5.105468	4.059291	-1.017166
6	5.049194	-4.138610	0.172214
6	4.890927	-3.982419	-1.253842
6	4.858918	3.763743	1.809437
6	4.735764	2.922025	2.979274
6	4.583350	-2.319143	-3.547947
6	4.440574	-1.002885	-4.136516
6	4.476170	0.333549	4.140667
6	4.337921	-1.101462	3.987916
6	4.172563	1.818440	-3.841225
6	4.045789	2.987900	-2.992214
6	4.044103	-3.404878	2.329160
6	3.889715	-4.011440	1.021391
6	3.801134	4.171994	-0.406830
6	3.680471	4.057138	1.033360
6	3.574087	-3.778824	-1.804940
6	3.420958	-2.963830	-2.993342
6	3.430608	2.457966	3.383018
6	3.302071	1.160321	4.008738
6	3.130702	-0.405634	-4.223249
6	2.996477	1.029321	-4.113446
6	3.025732	-1.672784	3.794587
6	2.879249	-2.860654	2.988270
6	2.740462	3.379927	-2.512160
6	2.618002	4.013104	-1.222402
6	2.567519	-4.122851	0.443407
6	2.409363	-4.044245	-0.985630
6	2.370917	3.858848	1.621020
6	2.246705	3.085915	2.828271
6	2.099106	-2.504354	-3.373117
6	1.953832	-1.233754	-4.031180
6	1.986528	0.561694	4.140207

6	1.849255	-0.869042	4.076603
6	1.681062	1.607098	-3.902026
6	1.553185	2.815931	-3.131285
6	1.554784	-3.269306	2.554154
6	1.399743	-3.942089	1.289526
6	1.305331	4.146653	-0.614243
6	1.183175	4.109045	0.822584
6	1.082655	-3.866613	-1.548895
6	0.928366	-3.124010	-2.778122
6	0.934274	2.643679	3.261307
6	0.806268	1.386315	3.964191
6	0.636351	-0.641784	-4.158287
6	0.501022	0.799207	-4.136780
6	0.532942	-1.454432	3.924635
6	0.387521	-2.693824	3.188475
6	0.244677	3.240283	-2.680210
6	0.122312	3.950231	-1.422315
6	0.078685	-4.095215	0.720756
6	-0.078685	-4.095230	-0.720673
6	-0.122312	3.950259	1.422232
6	-0.244677	3.240337	2.680141
6	-0.387521	-2.693888	-3.188420
6	-0.532942	-1.454511	-3.924606
6	-0.501022	0.799290	4.136762
6	-0.636351	-0.641700	4.158299
6	-0.806269	1.386235	-3.964221
6	-0.934274	2.643613	-3.261363
6	-0.928367	-3.123954	2.778186
6	-1.082655	-3.866583	1.548974
6	-1.183175	4.109029	-0.822670
6	-1.305331	4.146665	0.614156
6	-1.399743	-3.942115	-1.289446
6	-1.554784	-3.269357	-2.554088
6	-1.553185	2.815994	3.131226
6	-1.681062	1.607177	3.901992
6	-1.849256	-0.869125	-4.076586
6	-1.986529	0.561610	-4.140219
6	-1.953832	-1.233673	4.031204
6	-2.099106	-2.504286	3.373167
6	-2.246705	3.085858	-2.828335
6	-2.370917	3.858815	-1.621100
6	-2.409363	-4.044226	0.985712
6	-2.567519	-4.122860	-0.443323
6	-2.618002	4.013128	1.222318
6	-2.740462	3.379977	2.512089
6	-2.879249	-2.860714	-2.988212
6	-3.025733	-1.672861	-3.794553
6	-2.996477	1.029404	4.113423
6	-3.130702	-0.405549	4.223256
6	-3.302071	1.160239	-4.008762
6	-3.430609	2.457897	-3.383069
6	-3.420959	-2.963770	2.993402
6	-3.574087	-3.778789	1.805016
6	-3.680471	4.057116	-1.033443
6	-3.801134	4.172002	0.406744
6	-3.889715	-4.011462	-1.021309
6	-4.044103	-3.404926	-2.329091
6	-4.045788	2.987960	2.992152
6	-4.172562	1.818518	3.841187
6	-4.337922	-1.101544	-3.987894
6	-4.476171	0.333464	-4.140674
6	-4.440574	-1.002801	4.136535
6	-4.583350	-2.319071	3.547993
6	-4.735765	2.921964	-2.979334
6	-4.858919	3.763706	-1.809514
6	-4.890927	-3.982395	1.253923
6	-5.049194	-4.138615	-0.172130
6	-5.105468	4.059311	1.017082
6	-5.226090	3.494923	2.336472
6	-5.361813	-3.012024	-2.774577

6	-5.507832	-1.873971	-3.642136
6	-5.482613	1.248349	4.074075
6	-5.614667	-0.167101	4.260066
6	-5.789065	0.936454	-4.031447
6	-5.917971	2.253559	-3.481861
6	-5.904941	-2.787735	3.180360
6	-6.058669	-3.653492	2.051366
6	-6.171458	3.975546	-1.227303
6	-6.293164	4.162521	0.186551
6	-6.377483	-4.043005	-0.752267
6	-6.532177	-3.514912	-2.073862
6	-6.542549	3.119538	2.833375
6	-6.674759	2.020358	3.752924
6	-6.832264	-1.310343	-3.862493
6	-6.977537	0.099890	-4.114560
6	-6.942545	-0.769971	4.221348
6	-7.083964	-2.122774	3.715085
6	-7.241098	2.746442	-3.117294
6	-7.364834	3.657088	-1.992580
6	-7.390114	-3.904126	1.523067
6	-7.549719	-4.141741	0.098801
6	-7.606785	4.102229	0.800333
6	-7.718572	3.609429	2.160555
6	-7.857430	-3.167218	-2.548532
6	-7.995957	-2.073309	-3.491529
6	-7.989843	1.496728	4.072555
6	-8.109450	0.050272	4.378337
6	-8.295562	0.705369	-4.101979
6	-8.414433	2.106449	-3.639234
6	-8.391244	-2.648855	3.429948
6	-8.544219	-3.601485	2.323757
6	-8.665643	3.945926	-1.445332
6	-8.788244	4.206825	-0.012253
6	-8.866231	-4.121476	-0.486316
6	-9.022504	-3.655764	-1.859432
6	-9.018838	3.279038	2.697292
6	-9.125079	2.267304	3.689442
6	-9.306423	-1.528075	-3.767646
6	-9.428415	-0.161658	-4.129003
6	-9.383090	-0.628701	4.431139
6	-9.518363	-1.935905	3.990057
6	-9.688877	2.709833	-3.314657
6	-9.809724	3.607602	-2.268669
6	-9.838211	-3.956928	1.773329
6	-9.991652	-4.222479	0.426722
6	-10.075130	4.206599	0.675220
6	-10.187697	3.780087	1.978500
6	-10.325326	-3.329318	-2.433444
6	-10.463433	-2.324862	-3.361773
1	11.460909	-2.020928	3.708457
1	11.219427	-3.831934	2.042575
1	11.176435	3.686325	-2.448785
1	10.981059	4.457351	-0.108445
1	10.999774	-4.377882	-0.021624
1	10.727201	-3.905241	-2.415054
1	10.808034	3.955558	1.973969
1	10.594852	2.362997	3.828270
1	10.520912	-2.378653	-3.930685
1	10.282657	-0.065552	-4.711334
1	10.437696	0.264884	4.191983
1	10.130779	1.933018	-3.974964
1	-10.130774	1.933115	3.974944
1	-10.437696	0.264797	-4.191988
1	-10.282655	-0.065458	4.711347
1	-10.520911	-2.378574	3.930741
1	-10.594854	2.362916	-3.828314
1	-10.808035	3.955519	-1.974049
1	-10.727202	-3.905186	2.415133
1	-10.999774	-4.377877	0.021712
1	-10.981060	4.457354	0.108359

1	-11.176432	3.686384	2.448716
1	-11.219427	-3.831979	-2.042498
1	-11.460910	-2.021007	-3.708418

Nanotube (7,5) u08v06
B3LYP/STO-3G Energy: -7694.091499

6	10.530539	1.328741	-3.939967
6	10.409456	2.537593	-3.297289
6	10.305325	-3.195468	2.788188
6	10.173810	-3.940437	1.639362
6	10.118185	4.135446	-0.756612
6	9.981379	4.225763	0.614297
6	9.869543	-4.117755	-1.356400
6	9.737031	-3.518939	-2.596173
6	9.681994	2.846606	3.280649
6	9.547447	1.697909	4.043846
6	9.475986	-0.950642	-4.115936
6	9.364560	0.462886	-4.114120
6	9.270097	-1.289421	4.068798
6	9.147488	-2.519417	3.369539
6	9.115732	3.009594	-2.809461
6	8.979986	3.811991	-1.600308
6	8.877204	-4.108815	0.990778
6	8.735617	-4.224257	-0.458571
6	8.692752	4.033494	1.252852
6	8.550151	3.399120	2.567864
6	8.459772	-3.009444	-3.048567
6	8.339558	-1.773878	-3.853302
6	8.270244	1.036087	4.180522
6	8.141713	-0.438798	4.256307
6	8.059933	1.070563	-3.970688
6	7.939037	2.370088	-3.337384
6	7.838721	-2.968393	2.951696
6	7.707051	-3.792505	1.764720
6	7.671242	3.992589	-1.024677
6	7.529375	4.129818	0.414647
6	7.428045	-4.077910	-1.045563
6	7.291528	-3.486077	-2.365104
6	7.244499	2.973560	2.993954
6	7.104401	1.796859	3.832239
6	7.024052	-1.182151	-4.004277
6	6.888149	0.246958	-4.119987
6	6.821242	-1.018246	4.097425
6	6.673569	-2.315496	3.491352
6	6.622192	2.838074	-2.952175
6	6.487676	3.688386	-1.808210
6	6.385438	-4.000142	1.203516
6	6.244810	-4.181132	-0.209369
6	6.204261	4.033091	1.005001
6	6.061550	3.486844	2.319784
6	5.965535	-3.093231	-2.826702
6	5.833674	-1.960323	-3.693615
6	5.775265	1.232662	4.038492
6	5.635858	-0.181603	4.223091
6	5.569380	0.858020	-4.034453
6	5.440223	2.181002	-3.486343
6	5.349433	-2.796991	3.123000
6	5.209352	-3.679469	1.994787
6	5.167604	3.939661	-1.256275
6	5.027308	4.155064	0.163083
6	4.924675	-4.116371	-0.810025
6	4.787628	-3.601747	-2.153760
6	4.742448	3.136724	2.810084
6	4.601934	2.016967	3.717339
6	4.521149	-1.395322	-3.936463
6	4.390913	0.031031	-4.155483
6	4.320356	-0.783837	4.159519

6	4.178843	-2.130984	3.641548
6	4.130068	2.685676	-3.141193
6	3.996051	3.608577	-2.031679
6	3.896128	-3.937626	1.450266
6	3.755901	-4.194596	0.030476
6	3.716604	4.109764	0.763319
6	3.575287	3.626763	2.122261
6	3.478200	-3.247384	-2.646392
6	3.345456	-2.152082	-3.581924
6	3.291104	1.470875	3.969442
6	3.150529	0.056413	4.233599
6	3.083958	0.642848	-4.099626
6	2.954014	1.999806	-3.624794
6	2.866590	-2.625384	3.295020
6	2.725164	-3.568358	2.212795
6	2.682627	3.875694	-1.486610
6	2.542887	4.166281	-0.082994
6	2.439582	-4.144914	-0.571701
6	2.300521	-3.704186	-1.934511
6	2.256993	3.288489	2.621514
6	2.115027	2.229398	3.583895
6	2.030854	-1.597046	-3.844457
6	1.900388	-0.197183	-4.149192
6	1.830795	-0.547577	4.192279
6	1.689202	-1.912862	3.761424
6	1.637936	2.516953	-3.294720
6	1.503124	3.493254	-2.244591
6	1.404250	-3.845495	1.675521
6	1.262405	-4.175354	0.279660
6	1.222861	4.147756	0.522184
6	1.080819	3.743819	1.900545
6	0.983164	-3.376364	-2.448118
6	0.849415	-2.339643	-3.445564
6	0.796376	1.698100	3.872280
6	0.655594	0.301731	4.223641
6	0.588396	0.418082	-4.135791
6	0.458792	1.805861	-3.744902
6	0.373051	-2.431545	3.451322
6	0.232017	-3.441638	2.421874
6	0.190065	3.798621	-1.719041
6	0.051474	4.167684	-0.324468
6	-0.051474	-4.167709	-0.324163
6	-0.190065	-3.798750	-1.718763
6	-0.232017	3.441821	2.421624
6	-0.373051	2.431804	3.451146
6	-0.458792	-1.806140	-3.744772
6	-0.588396	-0.418389	-4.135761
6	-0.655595	-0.301416	4.223663
6	-0.796376	-1.697811	3.872403
6	-0.849415	2.339386	-3.445733
6	-0.983164	3.376181	-2.448364
6	-1.080818	-3.743675	1.900818
6	-1.222861	-4.147716	0.522488
6	-1.262405	4.175376	0.279354
6	-1.404250	3.845622	1.675241
6	-1.503124	-3.493422	-2.244337
6	-1.637935	-2.517199	-3.294538
6	-1.689203	1.913143	3.761285
6	-1.830796	0.547890	4.192240
6	-1.900388	0.196875	-4.149206
6	-2.030854	1.596760	-3.844572
6	-2.115027	-2.229130	3.584056
6	-2.256993	-3.288292	2.621754
6	-2.300521	3.704040	-1.934781
6	-2.439582	4.144871	-0.572005
6	-2.542887	-4.166288	-0.082689
6	-2.682627	-3.875806	-1.486326
6	-2.725165	3.568526	2.212535
6	-2.866591	2.625631	3.294829
6	-2.954014	-2.000076	-3.624649

6	-3.083958	-0.643152	-4.099580
6	-3.150530	-0.056098	4.233603
6	-3.291104	-1.470579	3.969549
6	-3.345456	2.151815	-3.582079
6	-3.478200	3.247186	-2.646628
6	-3.575286	-3.626604	2.122526
6	-3.716604	-4.109707	0.763620
6	-3.755901	4.194599	0.030168
6	-3.896129	3.937735	1.449977
6	-3.996051	-3.608729	-2.031415
6	-4.130068	-2.685911	-3.140997
6	-4.178844	2.131255	3.641392
6	-4.320357	0.784146	4.159461
6	-4.390912	-0.031339	-4.155481
6	-4.521149	1.395029	-3.936564
6	-4.601934	-2.016690	3.717485
6	-4.742447	-3.136514	2.810313
6	-4.787628	3.601586	-2.154024
6	-4.924675	4.116311	-0.810328
6	-5.027307	-4.155052	0.163388
6	-5.167604	-3.939755	-1.255986
6	-5.209353	3.679619	1.994517
6	-5.349434	2.797225	3.122796
6	-5.440223	-2.181261	-3.486184
6	-5.569380	-0.858319	-4.034391
6	-5.635858	0.181916	4.223077
6	-5.775265	-1.232363	4.038581
6	-5.833673	1.960048	-3.693758
6	-5.965534	3.093020	-2.826929
6	-6.061549	-3.486673	2.320040
6	-6.204260	-4.033017	1.005297
6	-6.244810	4.181117	-0.209677
6	-6.385439	4.000233	1.203221
6	-6.487676	-3.688520	-1.807939
6	-6.622192	-2.838293	-2.951966
6	-6.673570	2.315756	3.491181
6	-6.821243	1.018549	4.097349
6	-6.888149	-0.247263	-4.119970
6	-7.024051	1.181854	-4.004363
6	-7.104401	-1.796576	3.832371
6	-7.244497	-2.973340	2.994173
6	-7.291528	3.485900	-2.365360
6	-7.428045	4.077832	-1.045863
6	-7.529375	-4.129787	0.414951
6	-7.671242	-3.992664	-1.024383
6	-7.707051	3.792638	1.764440
6	-7.838722	2.968613	2.951477
6	-7.939038	-2.370335	-3.337210
6	-8.059933	-1.070857	-3.970611
6	-8.141715	0.439112	4.256274
6	-8.270244	-1.035780	4.180599
6	-8.339557	1.773591	-3.853432
6	-8.459771	3.009216	-3.048788
6	-8.550150	-3.398934	2.568116
6	-8.692751	-4.033403	1.253150
6	-8.735617	4.224224	-0.458883
6	-8.877205	4.108891	0.990474
6	-8.979987	-3.812108	-1.600026
6	-9.115733	-3.009802	-2.809240
6	-9.147489	2.519668	3.369352
6	-9.270097	1.289724	4.068703
6	-9.364560	-0.463191	-4.114088
6	-9.475986	0.950337	-4.116007
6	-9.547447	-1.697616	4.043976
6	-9.681993	-2.846369	3.280863
6	-9.737031	3.518741	-2.596430
6	-9.869543	4.117654	-1.356704
6	-9.981378	-4.225718	0.614609
6	-10.118185	-4.135499	-0.756306
6	-10.173810	3.940560	1.639070

6	-10.305325	3.195678	2.787952
6	-10.409456	-2.537838	-3.297104
6	-10.530539	-1.329034	-3.939873
1	11.521753	0.939098	-4.210500
1	11.310736	3.117204	-3.059253
1	11.300552	-2.990936	3.206789
1	11.070974	-4.334229	1.144446
1	11.121425	4.174473	-1.199904
1	10.878316	4.334496	1.237661
1	10.870396	-4.386685	-0.995211
1	10.636456	-3.323705	-3.194451
1	10.685041	3.253710	3.099529
1	10.447960	1.220045	4.450942
1	10.482464	-1.387026	-4.080806
1	10.280410	-0.899523	4.247660
1	-10.280410	0.899841	4.247596
1	-10.482464	1.386724	-4.080910
1	-10.447960	-1.219725	4.451040
1	-10.685039	-3.253488	3.099774
1	-10.636457	3.323457	-3.194692
1	-10.870396	4.386613	-0.995537
1	-10.878316	-4.334407	1.237981
1	-11.121427	-4.174557	-1.199595
1	-11.070975	4.334316	1.144124
1	-11.300552	2.991180	3.206570
1	-11.310736	-3.117431	-3.059026
1	-11.521753	-0.939411	-4.210437

Nanotube (7,5) u08v07
B3LYP/STO-3G Energy: -7769.386422

6	10.686151	-0.303926	4.051374
6	10.556488	-1.636234	3.740992
6	10.372971	2.346086	-3.613682
6	10.257820	3.360111	-2.691793
6	10.232302	-3.828797	1.695879
6	10.077520	-4.265956	0.395837
6	9.994510	4.298417	0.163544
6	9.877967	4.038058	1.516604
6	9.741907	-3.615888	-2.531484
6	9.596644	-2.701682	-3.561956
6	9.634923	1.947877	3.648603
6	9.522643	0.582384	4.010782
6	9.319246	0.179702	-4.349071
6	9.206750	1.547483	-3.986604
6	9.256236	-2.212524	3.404961
6	9.104870	-3.296167	2.443488
6	8.970167	3.693472	-2.090014
6	8.848376	4.176194	-0.717501
6	8.780037	-4.239290	-0.254406
6	8.619575	-3.962999	-1.685261
6	8.605891	3.667102	2.100921
6	8.495080	2.680698	3.196841
6	8.317041	-2.092415	-3.846914
6	8.187520	-0.686733	-4.296769
6	8.215664	-0.037071	4.043996
6	8.086206	-1.454867	3.766627
6	7.903775	2.093769	-3.680330
6	7.789022	3.194781	-2.742496
6	7.788484	-3.614383	1.950186
6	7.627744	-4.115112	0.595841
6	7.548515	4.191623	-0.095834
6	7.429001	3.958350	1.333050
6	7.307998	-3.657462	-2.189612
6	7.156079	-2.734681	-3.300019
6	7.181468	2.152816	3.511217
6	7.046274	0.801520	3.991444
6	6.869702	-0.080904	-4.274346

6	6.731015	1.329172	-4.019257
6	6.764765	-2.001240	3.530706
6	6.615547	-3.115980	2.644653
6	6.475705	3.545030	-2.236372
6	6.354502	4.082617	-0.915306
6	6.295320	-4.168884	0.017610
6	6.134761	-3.976911	-1.391072
6	6.109250	3.702261	1.896541
6	5.987678	2.829627	3.025766
6	5.824467	-2.237088	-3.625721
6	5.682483	-0.917202	-4.164371
6	5.726287	0.193727	4.080780
6	5.589626	-1.224406	3.892263
6	5.412454	1.894049	-3.768659
6	5.288574	3.036664	-2.903564
6	5.288248	-3.495833	2.192107
6	5.129457	-4.067214	0.878255
6	5.042410	4.179552	-0.301186
6	4.922565	4.026651	1.130240
6	4.808624	-3.759323	-1.937367
6	4.655127	-2.908874	-3.097957
6	4.677530	2.350422	3.421140
6	4.549051	1.028894	3.999511
6	4.367503	-0.313593	-4.239006
6	4.233762	1.121245	-4.082878
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6	3.982806	3.432177	-2.426870
6	3.862189	4.045688	-1.119373
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6	3.619311	3.816213	1.713851
6	3.497680	2.996502	2.899683
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6	3.196227	-1.140368	-4.079323
6	3.241273	0.428144	4.118382
6	3.104901	-1.005169	4.009899
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6	2.648804	-4.009337	1.151218
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6	2.326406	-3.851448	-1.683411
6	2.170470	-3.071628	-2.881638
6	2.186492	2.531715	3.310747
6	2.058782	1.256846	3.964213
6	1.877631	-0.540916	-4.174951
6	1.742674	0.889590	-4.108027
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6	1.488587	3.296853	-2.588888
6	1.366208	3.975369	-1.324019
6	1.321035	-4.143095	0.578531
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6	0.701252	-1.365486	-3.969424
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6	0.610489	-0.777222	4.104726
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6	0.060270	4.130195	-0.721835
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6	-1.877632	-0.540861	4.174957
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6	-3.650820	-4.054805	1.131842
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6	-4.808624	-3.759300	1.937417
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6	-8.215666	-0.037125	-4.043992
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6	-8.317043	-2.092362	3.846938
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6	-8.605892	3.667074	-2.100968
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6	-9.522644	0.582329	-4.010787
6	-9.634923	1.947828	-3.648628
6	-9.596645	-2.701634	3.561989
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6	-9.877967	4.038041	-1.516656
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1	10.326703	-0.247022	-4.436585
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1	-10.641007	2.357308	-3.491087
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B3LYP/STO-3G Energy: -7844.681174

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6	10.163068	-1.572233	-4.019767
6	10.110640	0.844489	4.196761
6	9.975926	-0.528124	4.290559
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6	9.738724	2.660107	-3.519151
6	9.697599	-3.120736	2.816142

6	9.575412	-3.818956	1.589774
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6	9.366127	4.164047	0.477769
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6	9.165610	-3.290710	-2.559637
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6	8.874172	-0.918824	-4.160605
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6	8.694642	-1.171075	4.081674
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6	-5.209323	-1.925436	3.705139
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6	-7.710798	-1.698562	3.822630
6	-7.854763	-2.880919	2.990779
6	-7.937536	3.404244	-2.383928
6	-8.060664	4.026072	-1.079076
6	-8.134821	-4.085447	0.437048
6	-8.265540	-3.990679	-1.004131
6	-8.343934	3.902773	1.766117
6	-8.464064	3.105095	3.007887
6	-8.565866	-2.476480	-3.412187
6	-8.694640	-1.166144	-4.083064
6	-8.733538	0.531271	4.259668
6	-8.874185	-0.923842	4.159449
6	-8.975005	1.685268	-3.851426
6	-9.112363	2.885725	-3.033512
6	-9.165616	-3.293809	2.555638
6	-9.307422	-3.946654	1.262208
6	-9.366123	4.164658	-0.472744
6	-9.479396	4.161392	0.941398
6	-9.575408	-3.817062	-1.594392
6	-9.697596	-3.117347	-2.819909
6	-9.738729	2.655867	3.522331
6	-9.868148	1.423581	4.140679
6	-9.975925	-0.522946	-4.291168
6	-10.110641	0.849553	-4.195707
6	-10.163080	-1.577078	4.017813
6	-10.301648	-2.723438	3.262108
6	-10.406658	3.366151	-2.557616
6	-10.530176	3.995450	-1.341363
6	-10.605144	-4.142330	0.618648
6	-10.735251	-4.101634	-0.748440
1	11.728957	-4.150438	1.209972
1	11.501652	-4.226614	-1.251310
1	11.522484	4.258231	0.955338
1	11.307267	3.128232	3.143631
1	11.304608	-3.127791	-3.087390
1	11.058266	-1.086320	-4.428918
1	11.112413	1.289908	4.245796
1	10.874484	-1.146935	4.411599
1	10.868690	1.068595	-4.410595
1	10.640641	3.250711	-3.312508
1	10.706777	-2.877689	3.171985
1	10.486365	4.124852	-1.371199
1	-10.486342	4.123242	1.376169

1	-10.706730	-2.873919	-3.175473
1	-10.640643	3.246722	3.316396
1	-10.868702	1.063270	4.411820
1	-10.874481	-1.141613	-4.412949
1	-11.112416	1.295028	-4.244193
1	-11.058282	-1.091654	4.427536
1	-11.304624	-3.131510	3.083549
1	-11.307263	3.132059	-3.139852
1	-11.522474	4.259452	-0.950213
1	-11.501650	-4.228177	1.246189
1	-11.728944	-4.149056	-1.215002

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B3LYP/STO-3G Energy: -7919.975737

6	10.880777	3.675801	-1.795749
6	10.759058	4.067131	-0.484648
6	10.580306	-4.304282	-0.301674
6	10.455976	-4.005412	-1.637736
6	10.455769	3.376139	2.434795
6	10.309571	2.462340	3.458030
6	10.179013	-1.986001	-3.862136
6	10.059821	-0.681825	-4.303794
6	9.983435	-0.404837	4.341722
6	9.836638	-1.752081	4.059093
6	9.820110	2.206345	-3.542930
6	9.712842	3.197412	-2.537305
6	9.543022	-3.866043	1.950972
6	9.420100	-4.229488	0.585807
6	9.462866	4.057982	0.191517
6	9.321488	3.759845	1.608608
6	9.164121	-3.644862	-2.216008
6	9.035556	-2.691707	-3.312254
6	9.014393	1.881320	3.764969
6	8.858900	0.502404	4.233137
6	8.787062	0.009771	-4.262778
6	8.677353	1.448907	-3.948700
6	8.553228	-2.302577	3.681328
6	8.415740	-3.389549	2.686231
6	8.408195	3.532715	-2.007554
6	8.286726	3.995103	-0.638701
6	8.111978	-4.233841	-0.031428
6	7.987271	-3.965100	-1.451274
6	8.008621	3.487597	2.138842
6	7.857009	2.558789	3.245590
6	7.733315	-2.159632	-3.626152
6	7.610808	-0.802603	-4.130308
6	7.547356	-0.087984	4.229383
6	7.394135	-1.510087	3.979137
6	7.365542	1.983653	-3.639347
6	7.234952	3.070823	-2.702691
6	7.094327	-3.671243	2.159274
6	6.945329	-4.148854	0.808811
6	6.969530	4.059471	-0.038604
6	6.830107	3.842101	1.370035
6	6.670898	-3.698560	-1.997150
6	6.542838	-2.817411	-3.118119
6	6.528328	2.081977	3.588505
6	6.373226	0.763104	4.120791
6	6.291501	-0.186669	-4.179227
6	6.170519	1.226017	-3.979472
6	6.061442	-2.039930	3.718374
6	5.912455	-3.160529	2.839564
6	5.917990	3.447595	-2.210145
6	5.788663	3.985399	-0.884729
6	5.622512	-4.208929	0.203237
6	5.488424	-4.023940	-1.215720
6	5.506825	3.634158	1.932889

6	5.357387	2.777620	3.080752
6	5.228149	-2.331292	-3.497688
6	5.104922	-1.014138	-4.073582
6	5.047759	0.179625	4.212538
6	4.893567	-1.248085	4.050148
6	4.860896	1.806475	-3.751026
6	4.736065	2.961555	-2.888878
6	4.592897	-3.523938	2.361364
6	4.448499	-4.097603	1.039600
6	4.476261	4.103136	-0.286011
6	4.337675	3.963533	1.148716
6	4.177772	-3.805227	-1.786699
6	4.049910	-2.975873	-2.967527
6	4.041204	2.330993	3.469733
6	3.887543	1.026130	4.080287
6	3.800790	-0.403246	-4.174580
6	3.679464	1.033010	-4.049802
6	3.577410	-1.799107	3.836891
6	3.426407	-2.977241	3.011445
6	3.430562	3.361293	-2.418070
6	3.301056	3.975308	-1.117035
6	3.137111	-4.185126	0.440729
6	3.001298	-4.076739	-0.992231
6	3.022502	3.775106	1.719240
6	2.874689	2.983177	2.914136
6	2.740923	-2.501943	-3.361929
6	2.616387	-1.220851	-4.007093
6	2.565717	0.445649	4.189348
6	2.410099	-0.981907	4.107171
6	2.370366	1.619660	-3.842797
6	2.245556	2.816787	-3.055404
6	2.105136	-3.355641	2.547345
6	1.959412	-4.002325	1.271337
6	1.984937	4.109607	-0.520059
6	1.846246	4.050401	0.910633
6	1.685007	-3.874418	-1.570819
6	1.555307	-3.116072	-2.787262
6	1.550855	2.550553	3.324481
6	1.397062	1.290625	4.005400
6	1.305273	-0.613132	-4.139726
6	1.182931	0.822937	-4.099345
6	1.085602	-1.546633	3.925694
6	0.933081	-2.768776	3.173397
6	0.933770	3.245345	-2.608822
6	0.804338	3.936704	-1.346677
6	0.641639	-4.128351	0.679385
6	0.504944	-4.106010	-0.760196
6	0.529149	3.901278	1.495294
6	0.382977	3.177154	2.740029
6	0.246125	-2.670165	-3.214227
6	0.122271	-1.421369	-3.935747
6	0.077638	0.719978	4.158812
6	-0.077638	-0.720032	4.158803
6	-0.122271	1.421419	-3.935730
6	-0.246125	2.670206	-3.214195
6	-0.382977	-3.177190	2.739990
6	-0.529149	-3.901298	1.495246
6	-0.504944	4.106019	-0.760146
6	-0.641639	4.128341	0.679436
6	-0.804338	-3.936686	-1.346726
6	-0.933770	-3.245311	-2.608861
6	-0.933081	2.768734	3.173430
6	-1.085602	1.546582	3.925712
6	-1.182931	-0.822885	-4.099355
6	-1.305272	0.613184	-4.139719
6	-1.397062	-1.290677	4.005385
6	-1.550855	-2.550596	3.324451
6	-1.555307	3.116108	-2.787224
6	-1.685007	3.874437	-1.570771
6	-1.846246	-4.050413	0.910583

6	-1.984938	-4.109600	-0.520109
6	-1.959413	4.002307	1.271386
6	-2.105135	3.355608	2.547386
6	-2.245556	-2.816748	-3.055438
6	-2.370366	-1.619611	-3.842817
6	-2.410099	0.981854	4.107184
6	-2.565717	-0.445703	4.189344
6	-2.616387	1.220902	-4.007079
6	-2.740923	2.501986	-3.361900
6	-2.874690	-2.983215	2.914100
6	-3.022503	-3.775128	1.719194
6	-3.001299	4.076751	-0.992181
6	-3.137111	4.185119	0.440780
6	-3.301056	-3.975293	-1.117083
6	-3.430561	-3.361262	-2.418111
6	-3.426406	2.977202	3.011481
6	-3.577409	1.799057	3.836913
6	-3.679463	-1.032959	-4.049816
6	-3.800789	0.403299	-4.174577
6	-3.887543	-1.026183	4.080276
6	-4.041205	-2.331037	3.469705
6	-4.049910	2.975910	-2.967491
6	-4.177772	3.805248	-1.786652
6	-4.337676	-3.963548	1.148667
6	-4.476262	-4.103131	-0.286061
6	-4.448499	4.097588	1.039651
6	-4.592897	3.523906	2.361407
6	-4.736065	-2.961518	-2.888915
6	-4.860896	-1.806427	-3.751048
6	-4.893566	1.248033	4.050164
6	-5.047759	-0.179678	4.212536
6	-5.104922	1.014189	-4.073570
6	-5.228150	2.331335	-3.497660
6	-5.357387	-2.777659	3.080719
6	-5.506826	-3.634181	1.932844
6	-5.488425	4.023953	-1.215670
6	-5.622512	4.208924	0.203289
6	-5.788664	-3.985386	-0.884778
6	-5.917990	-3.447565	-2.210187
6	-5.912454	3.160492	2.839604
6	-6.061442	2.039883	3.718400
6	-6.170518	-1.225967	-3.979489
6	-6.291500	0.186722	-4.179226
6	-6.373226	-0.763156	4.120783
6	-6.528329	-2.082022	3.588481
6	-6.542839	2.817449	-3.118084
6	-6.670899	3.698584	-1.997104
6	-6.830108	-3.842117	1.369987
6	-6.969531	-4.059468	-0.038654
6	-6.945329	4.148842	0.808863
6	-7.094326	3.671215	2.159321
6	-7.234951	-3.070788	-2.702730
6	-7.365541	-1.983607	-3.639374
6	-7.394134	1.510038	3.979158
6	-7.547356	0.087931	4.229386
6	-7.610808	0.802654	-4.130300
6	-7.733315	2.159677	-3.626127
6	-7.857010	-2.558829	3.245560
6	-8.008622	-3.487622	2.138799
6	-7.987272	3.965115	-1.451224
6	-8.111978	4.233839	-0.031375
6	-8.286726	-3.995092	-0.638751
6	-8.408195	-3.532687	-2.007598
6	-8.415739	3.389515	2.686275
6	-8.553227	2.302532	3.681358
6	-8.677351	-1.448857	-3.948721
6	-8.787061	-0.009719	-4.262782
6	-8.858900	-0.502457	4.233132
6	-9.014394	-1.881365	3.764947
6	-9.035556	2.691747	-3.312219

6	-9.164122	3.644886	-2.215961
6	-9.321489	-3.759862	1.608561
6	-9.462867	-4.057979	0.191466
6	-9.420099	4.229478	0.585861
6	-9.543021	3.866022	1.951023
6	-9.712842	-3.197378	-2.537346
6	-9.820110	-2.206302	-3.542963
6	-9.836638	1.752033	4.059120
6	-9.983434	0.404785	4.341731
6	-10.059821	0.681879	-4.303792
6	-10.179014	1.986048	-3.862114
6	-10.309572	-2.462382	3.458000
6	-10.455771	-3.376166	2.434753
6	-10.455978	4.005428	-1.637684
6	-10.580306	4.304284	-0.301619
6	-10.759059	-4.067120	-0.484700
6	-10.880778	-3.675776	-1.795796
1	11.872205	3.590626	-2.261934
1	11.659957	4.300936	0.097313
1	11.571990	-4.473429	0.140428
1	11.355158	-3.940799	-2.264047
1	11.461799	3.714461	2.155599
1	11.201762	2.087804	3.976354
1	11.175151	-2.442294	-3.798583
1	10.964643	-0.126276	-4.582503
1	10.989590	0.000810	4.508443
1	10.730559	-2.387145	4.008090
1	10.824562	1.867849	-3.827707
1	10.553271	-3.731986	2.358519
1	-10.553263	3.731967	2.358570
1	-10.824556	-1.867808	-3.827741
1	-10.730558	2.387098	4.008129
1	-10.989588	-0.000863	4.508452
1	-10.964641	0.126335	-4.582517
1	-11.175152	2.442342	-3.798558
1	-11.201763	-2.087854	3.976331
1	-11.461802	-3.714484	2.155552
1	-11.355159	3.940823	-2.263996
1	-11.571989	4.473430	0.140485
1	-11.659958	-4.300934	0.097258
1	-11.872205	-3.590599	-2.261983

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B3LYP/STO-3G Energy: -7995.270157

6	10.966580	-3.181834	2.628226
6	10.829457	-3.895128	1.462515
6	10.726850	4.151364	-0.856513
6	10.610648	4.206980	0.511932
6	10.506284	-3.973918	-1.534614
6	10.359577	-3.351564	-2.756836
6	10.333771	2.828613	3.181294
6	10.206649	1.682495	3.942472
6	10.053474	-0.802500	-4.342946
6	9.922358	0.573529	-4.413407
6	9.934834	-1.301633	3.946496
6	9.809688	-2.515496	3.229400
6	9.667066	3.160402	-2.915000
6	9.558664	3.863149	-1.688753
6	9.527216	-4.044944	0.814477
6	9.375741	-4.119007	-0.629995
6	9.320118	4.020351	1.170687
6	9.191872	3.381993	2.474702
6	9.067089	-2.853040	-3.194151
6	8.920863	-1.638885	-3.998568
6	8.927141	1.016785	4.086770
6	8.801935	-0.452665	4.152168
6	8.647350	1.217377	-4.181346

6	8.528729	2.523890	-3.497628
6	8.497057	-2.961397	2.811811
6	8.358950	-3.758054	1.608593
6	8.255462	4.040781	-1.086048
6	8.139701	4.146864	0.355667
6	8.060492	-3.977177	-1.204287
6	7.907683	-3.361701	-2.511265
6	7.887311	2.962513	2.922206
6	7.756850	1.781403	3.758132
6	7.615052	-1.052140	-4.138735
6	7.477956	0.388366	-4.260414
6	7.482879	-1.034643	3.999180
6	7.334357	-2.324324	3.373258
6	7.214698	2.946959	-3.053829
6	7.081306	3.756670	-1.870038
6	7.036104	-3.959810	1.053580
6	6.885797	-4.109237	-0.363004
6	6.825739	4.043735	0.958941
6	6.698796	3.480714	2.269196
6	6.580849	-2.973306	-2.956581
6	6.433858	-1.833201	-3.808427
6	6.433003	1.212964	3.970908
6	6.297840	-0.202160	4.140880
6	6.153170	0.982632	-4.136743
6	6.022498	2.292518	-3.573898
6	6.010095	-2.800250	3.002126
6	5.863812	-3.657855	1.859910
6	5.764347	3.984513	-1.292655
6	5.639828	4.170315	0.126558
6	5.559479	-4.036594	-0.951903
6	5.407637	-3.501223	-2.279425
6	5.382795	3.121664	2.767627
6	5.252443	1.998518	3.662494
6	5.113267	-1.277179	-4.038399
6	4.974500	0.145292	-4.247368
6	4.980935	-0.807642	4.077026
6	4.838318	-2.143143	3.541471
6	4.710374	2.781740	-3.197706
6	4.582097	3.675952	-2.066774
6	4.544684	-3.910428	1.319544
6	4.393954	-4.140719	-0.101614
6	4.331464	4.119287	0.741790
6	4.205369	3.621656	2.096041
6	4.091846	-3.153667	-2.761586
6	3.945469	-2.048058	-3.685856
6	3.943554	1.448276	3.925081
6	3.808643	0.029600	4.175069
6	3.665613	0.748068	-4.176289
6	3.533183	2.100460	-3.680566
6	3.525266	-2.636779	3.198222
6	3.378373	-3.562123	2.098476
6	3.276666	3.929196	-1.503399
6	3.151169	4.191853	-0.089281
6	3.075396	-4.089471	-0.692794
6	2.923998	-3.627724	-2.049923
6	2.895777	3.278744	2.605888
6	2.765149	2.207588	3.559477
6	2.628809	-1.499836	-3.932876
6	2.488214	-0.097311	-4.220854
6	2.493443	-0.576429	4.134489
6	2.351410	-1.934491	3.682465
6	2.220163	2.600836	-3.322486
6	2.090943	3.553781	-2.253511
6	2.056290	-3.829848	1.564401
6	1.904400	-4.135168	0.166950
6	1.838020	4.157503	0.528760
6	1.710790	3.736642	1.898657
6	1.600881	-3.298034	-2.548108
6	1.453343	-2.254277	-3.529037
6	1.449787	1.667943	3.850734

6	1.314722	0.272462	4.183303
6	1.171281	0.510804	-4.183754
6	1.037210	1.886449	-3.771250
6	1.031999	-2.449626	3.369614
6	0.884862	-3.438559	2.328134
6	0.779080	3.841498	-1.706276
6	0.653083	4.187465	-0.308595
6	0.582735	-4.123485	-0.427589
6	0.431568	-3.738958	-1.813698
6	0.400448	3.428356	2.432324
6	0.271261	2.408860	3.451367
6	0.137915	-1.726292	-3.816215
6	-0.002812	-0.334618	-4.188985
6	0.002813	-0.334427	4.189001
6	-0.137915	-1.726117	3.816294
6	-0.271261	2.408703	-3.451477
6	-0.400448	3.428244	-2.432480
6	-0.431569	-3.738874	1.813869
6	-0.582736	-4.123465	0.427777
6	-0.653084	4.187479	0.308404
6	-0.779080	3.841576	1.706101
6	-0.884862	-3.438665	-2.327976
6	-1.031999	-2.449780	-3.369502
6	-1.037210	1.886621	3.771164
6	-1.171280	0.510996	4.183732
6	-1.314721	0.272271	-4.183316
6	-1.449786	1.667767	-3.850810
6	-1.453343	-2.254116	3.529141
6	-1.600881	-3.297917	2.548259
6	-1.710791	3.736555	-1.898828
6	-1.838021	4.157477	-0.528950
6	-1.904401	-4.135175	-0.166761
6	-2.056290	-3.829918	-1.564225
6	-2.090943	3.553883	2.253349
6	-2.220162	2.600987	3.322368
6	-2.351409	-1.934659	-3.682378
6	-2.493441	-0.576618	-4.134464
6	-2.488213	-0.097118	4.220860
6	-2.628808	-1.499656	3.932946
6	-2.765149	2.207425	-3.559578
6	-2.895778	3.278623	-2.606038
6	-2.923999	-3.627629	2.050089
6	-3.075397	-4.089437	0.692981
6	-3.151170	4.191855	0.089090
6	-3.276667	3.929263	1.503220
6	-3.378373	-3.562218	-2.098313
6	-3.525266	-2.636925	-3.198103
6	-3.533182	2.100628	3.680472
6	-3.665612	0.748259	4.176258
6	-3.808642	0.029409	-4.175073
6	-3.943553	1.448096	-3.925149
6	-3.945469	-2.047888	3.685951
6	-4.091846	-3.153539	2.761730
6	-4.205370	3.621558	-2.096206
6	-4.331465	4.119250	-0.741978
6	-4.393955	-4.140711	0.101803
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6	-4.582098	3.676045	2.066607
6	-4.710374	2.781886	3.197581
6	-4.838317	-2.143305	-3.541376
6	-4.980934	-0.807829	-4.076993
6	-4.974499	0.145486	4.247365
6	-5.113266	-1.276993	4.038460
6	-5.252442	1.998349	-3.662587
6	-5.382796	3.121535	-2.767771
6	-5.407638	-3.501115	2.279585
6	-5.559480	-4.036546	0.952087
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6	-6.297839	-0.202350	-4.140876
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6	-6.433858	-1.833025	3.808513
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6	-6.698796	3.480606	-2.269355
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6	-6.885798	-4.109215	0.363191
6	-7.036105	-3.959854	-1.053401
6	-7.081306	3.756752	1.869868
6	-7.214698	2.947098	3.053698
6	-7.334356	-2.324478	-3.373157
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6	-7.477955	0.388561	4.260402
6	-7.615051	-1.051949	4.138788
6	-7.756850	1.781229	-3.758217
6	-7.887312	2.962375	-2.922342
6	-7.907685	-3.361581	2.511417
6	-8.060494	-3.977115	1.204467
6	-8.139702	4.146841	-0.355855
6	-8.255463	4.040825	1.085865
6	-8.358951	-3.758124	-1.608424
6	-8.497056	-2.961524	-2.811679
6	-8.528729	2.524051	3.497518
6	-8.647349	1.217569	4.181298
6	-8.801934	-0.452856	-4.152155
6	-8.927140	1.016597	-4.086822
6	-8.920863	-1.638699	3.998647
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6	-9.375743	-4.118970	0.630181
6	-9.527217	-4.044976	-0.814295
6	-9.558664	3.863221	1.688579
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6	-9.922356	0.573733	4.413390
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6	-10.206648	1.682311	-3.942553
6	-10.333771	2.828461	-3.181423
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1	11.962798	-2.991506	3.051102
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1	11.514080	4.296430	1.128996
1	11.511337	-4.241857	-1.184501
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1	10.822611	1.190231	-4.532694
1	10.944564	-0.912404	4.129315
1	10.672447	2.915043	-3.280395
1	-10.672444	2.915195	3.280269
1	-10.944560	-0.912597	-4.129287
1	-10.822609	1.190441	4.532650
1	-11.053907	-1.249127	4.407344
1	-11.108476	1.207225	-4.350031
1	-11.333134	3.243538	-2.998331
1	-11.250336	-3.133398	3.360273
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1	-11.716285	4.191284	1.332698
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Nanotube (7,5) u08v11
B3LYP/STO-3G Energy: -8070.565078

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C	10.632602	4.163754	0.388009
C	10.493727	3.881502	1.738580
C	10.365848	-3.621903	-2.405801
C	10.237555	-2.708351	-3.445022
C	10.186030	1.839359	3.937576
C	10.047177	0.522246	4.366829
C	9.984564	0.172372	-4.230465
C	9.878096	1.542204	-3.844037
C	9.761725	-2.364520	3.593875
C	9.639170	-3.364388	2.580038
C	9.636577	3.640401	-1.898701
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C	9.235416	-3.964386	-1.578120
C	9.210420	3.534207	2.299577
C	9.063231	2.563762	3.402314
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C	8.853627	-0.683532	-4.194859
C	8.775980	-0.146052	4.320341
C	8.642656	-1.593424	3.995406
C	8.579182	2.088503	-3.537625
C	8.460633	3.167134	-2.575141
C	8.334354	-3.673559	2.050601
C	8.203876	-4.142690	0.684770
C	8.192839	4.103990	0.093195
C	8.048653	3.847757	1.513731
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C	7.166210	-3.186626	2.746453
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C	6.136006	-1.330806	4.029633
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C	5.431397	-3.758604	-1.889905
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C	4.398025	-4.186624	0.332022
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H	-11.565544	4.484335	-0.058727
H	-11.790523	3.754919	2.290945
H	-11.830470	-3.785406	-2.087228
H	-12.035746	-2.001899	-3.785497

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B3LYP/STO-3G Energy: -8145.863738

6	-11.179129	-1.411357	-3.829906
6	-11.045985	-2.615179	-3.170366
6	-10.893402	3.204214	2.841068
6	-10.779127	3.935929	1.676171
6	-10.718710	-4.178017	-0.614138
6	-10.565656	-4.249642	0.762059
6	-10.511250	4.074266	-1.324089
6	-10.391347	3.455780	-2.562406
6	-10.241370	-2.832445	3.405086
6	-10.102736	-1.667328	4.154040
6	-10.137426	0.870309	-4.056928
6	-10.021549	-0.551862	-4.036643
6	-9.836878	1.322760	4.141850
6	-9.728965	2.550794	3.419293
6	-9.750010	-3.078121	-2.699501
6	-9.596578	-3.868477	-1.471874
6	-9.496533	4.105586	1.014994
6	-9.372565	4.200695	-0.447271
6	-9.277145	-4.047769	1.380482
6	-9.121331	-3.389533	2.692474
6	-9.124774	2.948802	-3.022670
6	-9.008820	1.696131	-3.815998
6	-8.834170	-1.001412	4.267440
6	-8.710250	0.481673	4.321948
6	-8.716909	-1.149650	-3.894138
6	-8.583646	-2.438767	-3.242678
6	-8.430727	2.993463	2.975178
6	-8.316800	3.799191	1.774930
6	-8.282396	-4.027338	-0.907843

6	-8.123145	-4.142285	0.529445
6	-8.072437	4.042528	-1.044905
6	-7.948783	3.432981	-2.354725
6	-7.812728	-2.946977	3.090588
6	-7.667156	-1.760029	3.908599
6	-7.688598	1.107159	-3.968426
6	-7.547341	-0.321252	-4.067099
6	-7.389487	1.061542	4.134917
6	-7.253502	2.350733	3.510682
6	-7.257006	-2.896697	-2.867217
6	-7.105391	-3.732327	-1.712029
6	-6.999612	4.005927	1.196096
6	-6.876372	4.167828	-0.224311
6	-6.788960	-4.036926	1.102932
6	-6.632905	-3.470498	2.413456
6	-6.625143	3.045875	-2.830653
6	-6.499210	1.895516	-3.689670
6	-6.337139	-1.192158	4.098723
6	-6.201546	0.234398	4.264486
6	-6.227757	-0.925348	-3.994950
6	-6.087604	-2.249132	-3.426196
6	-5.939303	2.834379	3.125197
6	-5.817381	3.706938	1.975122
6	-5.784274	-3.974139	-1.175708
6	-5.627066	-4.169076	0.254558
6	-5.570589	4.103012	-0.838190
6	-5.448434	3.565443	-2.183667
6	-5.317915	-3.110788	2.882494
6	-5.171675	-1.971021	3.775702
6	-5.193954	1.333666	-3.936479
6	-5.059624	-0.098800	-4.136025
6	-4.895582	0.837690	4.172636
6	-4.764671	2.179191	3.632254
6	-4.775673	-2.738344	-3.084907
6	-4.624626	-3.643466	-1.964205
6	-4.514872	3.954863	1.409252
6	-4.392121	4.190787	-0.013532
6	-4.311182	-4.102666	0.837025
6	-4.155427	-3.600420	2.183913
6	-4.141697	3.204803	-2.682156
6	-4.014360	2.099653	-3.601498
6	-3.857075	-1.415187	3.998850
6	-3.717792	0.000312	4.241079
6	-3.745431	-0.703633	-4.084130
6	-3.603500	-2.052325	-3.592995
6	-3.454051	2.672434	3.262332
6	-3.328773	3.601544	2.165685
6	-3.299792	-3.899397	-1.431915
6	-3.142575	-4.171711	-0.023415
6	-3.079380	4.142814	-0.630455
6	-2.955256	3.682686	-1.994611
6	-2.830437	-3.256834	2.666292
6	-2.681651	-2.178168	3.618109
6	-2.700616	1.551188	-3.878734
6	-2.567910	0.137884	-4.167670
6	-2.402456	0.607440	4.183714
6	-2.271661	1.977621	3.728797
6	-2.285686	-2.561387	-3.277747
6	-2.135239	-3.529749	-2.206894
6	-2.021227	3.880287	1.613196
6	-1.898543	4.192739	0.200282
6	-1.823748	-4.144068	0.564236
6	-1.668219	-3.716173	1.944378
6	-1.650790	3.355157	-2.517804
6	-1.525055	2.298497	-3.505733
6	-1.370260	-1.639306	3.880416
6	-1.230684	-0.232141	4.208488
6	-1.260437	-0.469054	-4.155842
6	-1.119817	-1.851411	-3.743336
6	-0.967652	2.491104	3.390411

6	-0.842169	3.485380	2.344534
6	-0.819319	-3.813642	-1.689193
6	-0.662780	-4.161977	-0.294149
6	-0.593450	4.172147	-0.417649
6	-0.469162	3.785537	-1.804261
6	-0.350160	-3.395193	2.440663
6	-0.199641	-2.373216	3.449499
6	-0.215274	1.763585	-3.807264
6	-0.082633	0.375209	-4.178447
6	0.082633	0.375182	4.178450
6	0.215274	1.763560	3.807276
6	0.199641	-2.373194	-3.449513
6	0.350160	-3.395177	-2.440685
6	0.469162	3.785525	1.804286
6	0.593450	4.172144	0.417677
6	0.662780	-4.161979	0.294123
6	0.819319	-3.813654	1.689169
6	0.842169	3.485395	-2.344511
6	0.967652	2.491126	-3.390395
6	1.119817	-1.851435	3.743324
6	1.260437	-0.469081	4.155839
6	1.230684	-0.232114	-4.208489
6	1.370260	-1.639281	-3.880426
6	1.525055	2.298474	3.505748
6	1.650790	3.355141	2.517827
6	1.668219	-3.716160	-1.944401
6	1.823748	-4.144065	-0.564262
6	1.898543	4.192740	-0.200255
6	2.021227	3.880297	-1.613171
6	2.135239	-3.529763	2.206872
6	2.285686	-2.561408	3.277731
6	2.271661	1.977645	-3.728784
6	2.402456	0.607467	-4.183709
6	2.567910	0.137857	4.167672
6	2.700616	1.551163	3.878744
6	2.681651	-2.178144	-3.618122
6	2.830437	-3.256816	-2.666313
6	2.955256	3.682674	1.994635
6	3.079380	4.142810	0.630482
6	3.142575	-4.171712	0.023388
6	3.299792	-3.899406	1.431890
6	3.328773	3.601558	-2.165661
6	3.454051	2.672455	-3.262315
6	3.603501	-2.052349	3.592982
6	3.745432	-0.703660	4.084126
6	3.717792	0.000339	-4.241078
6	3.857075	-1.415161	-3.998858
6	4.014361	2.099630	3.601511
6	4.141697	3.204786	2.682177
6	4.155427	-3.600407	-2.183936
6	4.311182	-4.102661	-0.837052
6	4.392121	4.190787	0.013559
6	4.514872	3.954873	-1.409226
6	4.624626	-3.643479	1.964182
6	4.775673	-2.738364	3.084890
6	4.764670	2.179214	-3.632240
6	4.895582	0.837717	-4.172630
6	5.059625	-0.098827	4.136023
6	5.193954	1.333641	3.936486
6	5.171675	-1.970997	-3.775714
6	5.317914	-3.110769	-2.882514
6	5.448434	3.565429	2.183690
6	5.570590	4.103007	0.838216
6	5.627066	-4.169076	-0.254585
6	5.784274	-3.974148	1.175683
6	5.817381	3.706951	-1.975099
6	5.939302	2.834400	-3.125178
6	6.087605	-2.249155	3.426181
6	6.227757	-0.925374	3.994943
6	6.201545	0.234426	-4.264484

6	6.337138	-1.192131	-4.098730
6	6.499210	1.895492	3.689681
6	6.625143	3.045857	2.830672
6	6.632905	-3.470483	-2.413479
6	6.788960	-4.036919	-1.102958
6	6.876372	4.167827	0.224337
6	6.999612	4.005935	-1.196070
6	7.105391	-3.732339	1.712004
6	7.257006	-2.896716	2.867197
6	7.253501	2.350756	-3.510667
6	7.389487	1.061569	-4.134910
6	7.547341	-0.321278	4.067095
6	7.688598	1.107133	3.968432
6	7.667156	-1.760004	-3.908610
6	7.812728	-2.946957	-3.090607
6	7.948783	3.432966	2.354747
6	8.072437	4.042522	1.044930
6	8.123145	-4.142283	-0.529472
6	8.282396	-4.027345	0.907816
6	8.316799	3.799203	-1.774907
6	8.430727	2.993482	-2.975160
6	8.583646	-2.438788	3.242661
6	8.716909	-1.149676	3.894130
6	8.710249	0.481702	-4.321946
6	8.834170	-1.001385	-4.267447
6	9.008820	1.696106	3.816010
6	9.124775	2.948783	3.022688
6	9.121331	-3.389515	-2.692496
6	9.277144	-4.047761	-1.380508
6	9.372565	4.200694	0.447297
6	9.496533	4.105594	-1.014969
6	9.596578	-3.868489	1.471849
6	9.750010	-3.078140	2.699480
6	9.728965	2.550817	-3.419278
6	9.836877	1.322788	-4.141844
6	10.021549	-0.551889	4.036641
6	10.137425	0.870283	4.056938
6	10.102736	-1.667300	-4.154051
6	10.241370	-2.832422	-3.405104
6	10.391348	3.455765	2.562428
6	10.511251	4.074259	1.324115
6	10.565655	-4.249639	-0.762087
6	10.718710	-4.178024	0.614110
6	10.779126	3.935941	-1.676148
6	10.893402	3.204234	-2.841050
6	11.045985	-2.615200	3.170349
6	11.179129	-1.411381	3.829897
1	-12.176666	-1.025182	-4.081457
1	-11.945208	-3.185241	-2.903391
1	-11.884485	2.992997	3.266050
1	-11.687031	4.306005	1.182579
1	-11.729209	-4.215210	-1.040652
1	-11.458598	-4.340116	1.394003
1	-11.511448	4.331870	-0.952948
1	-11.301101	3.238195	-3.136907
1	-11.247477	-3.236526	3.234319
1	-11.004568	-1.184033	4.551786
1	-11.146714	1.299286	-4.010741
1	-10.844972	0.932484	4.332538
1	10.844971	0.932515	-4.332537
1	11.146714	1.299260	4.010761
1	11.004567	-1.184004	-4.551794
1	11.247477	-3.236503	-3.234337
1	11.301102	3.238177	3.136927
1	11.511448	4.331866	0.952976
1	11.458597	-4.340109	-1.394032
1	11.729208	-4.215221	1.040623
1	11.687031	4.306015	-1.182555
1	11.884485	2.993019	-3.266033
1	11.945208	-3.185260	2.903370

1 12.176665 -1.025209 4.081451

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6	-11.237867	-0.355310	-4.159540
6	-11.113415	-1.687699	-3.828052
6	-11.029320	2.395178	3.478026
6	-10.901545	3.399541	2.540320
6	-10.818201	-3.852018	-1.751005
6	-10.681548	-4.273823	-0.437827
6	-10.598777	4.299531	-0.322014
6	-10.464146	4.019338	-1.675692
6	-10.386675	-3.584215	2.484222
6	-10.255680	-2.651530	3.508514
6	-10.192437	1.904376	-3.781254
6	-10.077209	0.524860	-4.124827
6	-9.988084	0.240335	4.265598
6	-9.871498	1.611436	3.882622
6	-9.823092	-2.260142	-3.474971
6	-9.685190	-3.337782	-2.488739
6	-9.610974	3.728366	1.958359
6	-9.470057	4.193978	0.571107
6	-9.399629	-4.242426	0.226282
6	-9.258517	-3.943705	1.664324
6	-9.191582	3.644010	-2.236332
6	-9.066130	2.637093	-3.323158
6	-8.987452	-2.041417	3.802784
6	-8.863440	-0.622651	4.236909
6	-8.774397	-0.094171	-4.125088
6	-8.649804	-1.507654	-3.823671
6	-8.567970	2.149034	3.581155
6	-8.440242	3.234710	2.628141
6	-8.377927	-3.641421	-1.969583
6	-8.235915	-4.121189	-0.607693
6	-8.163059	4.191211	-0.032376
6	-8.023909	3.937476	-1.453391
6	-7.954289	-3.623619	2.177471
6	-7.817207	-2.686718	3.274387
6	-7.744665	2.102388	-3.606228
6	-7.602712	0.746554	-4.066015
6	-7.540697	-0.018455	4.218935
6	-7.397286	1.387020	3.947049
6	-7.328361	-2.051107	-3.562129
6	-7.191477	-3.154785	-2.657848
6	-7.116558	3.578575	2.136104
6	-6.976892	4.098327	0.806424
6	-6.908620	-4.171182	-0.011304
6	-6.767316	-3.959953	1.401605
6	-6.694579	3.680576	-1.997341
6	-6.558256	2.788706	-3.120189
6	-6.488876	-2.190590	3.617551
6	-6.354323	-0.855256	4.144417
6	-6.283838	0.139252	-4.134808
6	-6.151370	-1.285767	-3.922799
6	-6.078194	1.949022	3.712439
6	-5.943083	3.086482	2.826128
6	-5.876409	-3.531101	-2.186231
6	-5.736475	-4.086394	-0.852628
6	-5.663457	4.189517	0.211224
6	-5.525259	4.014109	-1.225292
6	-5.456779	-3.737480	1.961907
6	-5.319855	-2.865041	3.118421
6	-5.249692	2.304523	-3.487717
6	-5.113378	0.970371	-4.045904
6	-5.046690	-0.252803	4.224520
6	-4.909465	1.182170	4.047636
6	-4.843840	-1.851251	-3.703647

6	-4.707311	-3.014529	-2.850904
6	-4.634256	3.467934	2.357771
6	-4.495226	4.060401	1.044228
6	-4.427656	-4.177514	-0.257969
6	-4.287206	-4.037085	1.174597
6	-4.213077	3.789228	-1.784556
6	-4.074563	2.955103	-2.954165
6	-4.007737	-2.389245	3.490541
6	-3.870427	-1.083236	4.088386
6	-3.800477	0.367652	-4.134489
6	-3.665516	-1.062128	-4.004138
6	-3.594757	1.749646	3.830620
6	-3.457093	2.928713	3.011186
6	-3.389547	-3.403573	-2.386802
6	-3.249521	-4.028275	-1.094225
6	-3.175360	4.168197	0.450403
6	-3.034924	4.071846	-0.983695
6	-2.967437	-3.832454	1.743186
6	-2.828446	-3.033292	2.939394
6	-2.756965	2.490482	-3.346048
6	-2.620945	1.198416	-3.984419
6	-2.553596	-0.485805	4.201710
6	-2.417333	0.954316	4.115369
6	-2.351177	-1.640174	-3.814208
6	-2.214761	-2.851506	-3.027878
6	-2.142866	3.336764	2.563753
6	-2.004023	4.001437	1.280233
6	-1.936813	-4.158138	-0.504321
6	-1.796949	-4.097669	0.940497
6	-1.723759	3.885681	-1.558292
6	-1.585569	3.114902	-2.781238
6	-1.518930	-2.583907	3.344859
6	-1.382352	-1.307439	4.023084
6	-1.313430	0.604070	-4.112742
6	-1.178980	-0.838952	-4.067900
6	-1.109422	1.533746	3.934841
6	-0.972442	2.763989	3.181944
6	-0.905652	-3.265706	-2.586627
6	-0.766486	-3.961974	-1.325791
6	-0.692525	4.137656	0.692780
6	-0.551784	4.117456	-0.745188
6	-0.484765	-3.919412	1.516763
6	-0.344820	-3.187692	2.754040
6	-0.272677	2.669577	-3.192401
6	-0.135680	1.420995	-3.902707
6	-0.068590	-0.716750	4.162573
6	0.068591	0.719864	4.162037
6	0.135681	-1.423922	-3.901645
6	0.272677	-2.671973	-3.190407
6	0.344819	3.189753	2.751658
6	0.484764	3.920546	1.513834
6	0.551784	-4.118017	-0.742110
6	0.692525	-4.137138	0.695873
6	0.766486	3.960975	-1.328751
6	0.905652	3.263763	-2.589066
6	0.972443	-2.761606	3.184007
6	1.109423	-1.530801	3.935985
6	1.178981	0.835902	-4.068525
6	1.313431	-0.607153	-4.112290
6	1.382352	1.310450	4.022107
6	1.518929	2.586411	3.342928
6	1.585569	-3.116990	-2.778911
6	1.723759	-3.886853	-1.555388
6	1.796948	4.098371	0.937434
6	1.936811	4.157755	-0.507429
6	2.004023	-4.000478	1.283223
6	2.142867	-3.334843	2.566245
6	2.214761	2.849232	-3.030006
6	2.351177	1.637313	-3.815430
6	2.417334	-0.951235	4.116079

6	2.553596	0.488949	4.201346
6	2.620946	-1.201404	-3.983523
6	2.756965	-2.492993	-3.344188
6	2.828444	3.035493	2.937128
6	2.967435	3.833759	1.740322
6	3.034924	-4.072586	-0.980652
6	3.175361	-4.167860	0.453518
6	3.249519	4.027450	-1.097235
6	3.389547	3.401779	-2.389343
6	3.457095	-2.926456	3.013371
6	3.594759	-1.746777	3.831924
6	3.665517	1.059125	-4.004928
6	3.800478	-0.370751	-4.134213
6	3.870427	1.086297	4.087577
6	4.007735	2.391860	3.488758
6	4.074563	-2.957320	-2.951959
6	4.213077	-3.790569	-1.781725
6	4.287203	4.037965	1.171581
6	4.427654	4.177319	-0.261091
6	4.495227	-4.059617	1.047261
6	4.634259	-3.466165	2.360360
6	4.707311	3.012387	-2.853152
6	4.843841	1.848472	-3.705025
6	4.909467	-1.179137	4.048515
6	5.046690	0.255968	4.224329
6	5.113378	-0.973404	-4.045179
6	5.249692	-2.307141	-3.485997
6	5.319852	2.867380	3.116283
6	5.456775	3.738953	1.959116
6	5.525259	-4.015031	-1.222293
6	5.663457	-4.189360	0.214354
6	5.736473	4.085752	-0.855680
6	5.876409	3.529458	-2.188865
6	5.943086	-3.084359	2.828429
6	6.078197	-1.946237	3.713889
6	6.151371	1.282825	-3.923753
6	6.283839	-0.142353	-4.134701
6	6.354322	0.858364	4.143778
6	6.488874	2.193304	3.615917
6	6.558255	-2.791050	-3.118109
6	6.694579	-3.682079	-1.994594
6	6.767312	3.961009	1.398649
6	6.908617	4.171175	-0.014418
6	6.976893	-4.097721	0.809484
6	7.116561	-3.576969	2.138773
6	7.191477	3.152788	-2.660199
6	7.328362	2.048433	-3.563653
6	7.397289	-1.384057	3.948077
6	7.540698	0.021620	4.218919
6	7.602713	-0.749604	-4.065456
6	7.744664	-2.105096	-3.604662
6	7.817203	2.689181	3.272385
6	7.954284	3.625261	2.174768
6	8.023909	-3.938573	-1.450453
6	8.163059	-4.191238	-0.029247
6	8.235913	4.120735	-0.610769
6	8.377926	3.639941	-1.972297
6	8.440246	-3.232730	2.630548
6	8.567975	-2.146341	3.582749
6	8.649805	1.504785	-3.824787
6	8.774398	0.091077	-4.125152
6	8.863439	0.625833	4.236442
6	8.987449	2.044278	3.801264
6	9.066129	-2.639591	-3.321193
6	9.191581	-3.645696	-2.233616
6	9.258511	3.944966	1.661383
6	9.399625	4.242603	0.223117
6	9.470058	-4.193549	0.574234
6	9.610978	-3.726888	1.961134
6	9.685189	3.335913	-2.491223

6	9.823093	2.257533	-3.476646
6	9.871502	-1.608513	3.883808
6	9.988086	-0.237127	4.265765
6	10.077210	-0.527953	-4.124427
6	10.192437	-1.907214	-3.779830
6	10.255676	2.654177	3.506543
6	10.386670	3.586096	2.481555
6	10.464145	-4.020605	-1.672698
6	10.598778	-4.299778	-0.318809
6	10.681544	4.273502	-0.441015
6	10.818199	3.850706	-1.753875
6	10.901550	-3.397617	2.542839
6	11.029325	-2.392549	3.479789
6	11.113417	1.684824	-3.829294
6	11.237869	0.352189	-4.159788
1	-12.231846	0.085780	-4.317224
1	-12.015826	-2.304477	-3.727560
1	-12.025148	2.086022	3.824786
1	-11.803458	3.887141	2.148258
1	-11.823447	-3.775381	-2.184642
1	-11.581766	-4.520241	0.139917
1	-11.603183	4.456539	0.091525
1	-11.366781	3.959629	-2.297551
1	-11.390871	-3.927978	2.204795
1	-11.161302	-2.283861	4.008227
1	-11.201875	2.311168	-3.639253
1	-10.998321	-0.182583	4.339618
1	10.998327	0.185849	4.339453
1	11.201878	-2.313897	-3.637514
1	11.161298	2.286884	4.006532
1	11.390862	3.929655	2.201874
1	11.366778	-3.961366	-2.294603
1	11.603183	-4.456476	0.094848
1	11.581762	4.520358	0.136544
1	11.823446	3.773745	-2.187454
1	11.803464	-3.885505	2.151136
1	12.025157	-2.083127	3.826308
1	12.015828	2.301677	-3.729259
1	12.231851	-0.089018	-4.317136

Nanotube (7,5) u09v02
B3LYP/STO-3G Energy: -8296.460098

6	-11.388421	-4.018753	-0.724619
6	-11.263451	-4.043388	0.647673
6	-11.088851	4.070167	-1.415356
6	-10.969341	3.421115	-2.626786
6	-10.951439	-2.596215	3.273019
6	-10.801889	-1.437561	4.017877
6	-10.696955	0.882684	-4.232407
6	-10.578074	-0.498380	-4.310262
6	-10.473392	1.560260	4.103442
6	-10.328414	2.788488	3.466794
6	-10.333847	-3.081149	-2.810259
6	-10.225187	-3.770078	-1.566903
6	-10.044101	4.263192	0.868895
6	-9.928157	4.245294	-0.553944
6	-9.970309	-3.863140	1.291185
6	-9.824632	-3.189385	2.585681
6	-9.684224	2.927714	-3.094783
6	-9.558034	1.705989	-3.901368
6	-9.512289	-0.801808	4.158141
6	-9.354866	0.662518	4.239671
6	-9.311951	-1.151362	-4.093339
6	-9.200538	-2.461994	-3.401120
6	-9.054630	3.216066	2.953482
6	-8.921688	3.999988	1.695103
6	-8.923561	-3.944726	-0.969697

6	-8.798990	-4.019352	0.473733
6	-8.626571	4.077568	-1.151765
6	-8.507120	3.434729	-2.446421
6	-8.512623	-2.780656	3.012728
6	-8.357432	-1.589614	3.826924
6	-8.257913	1.107462	-4.055918
6	-8.135302	-0.332690	-4.176917
6	-8.044303	1.226333	4.063376
6	-7.892475	2.526211	3.440837
6	-7.883745	-2.888429	-2.958597
6	-7.749676	-3.683674	-1.767172
6	-7.597988	4.123034	1.106138
6	-7.453975	4.220681	-0.321878
6	-7.476277	-3.920658	1.065553
6	-7.332560	-3.332939	2.364638
6	-7.188509	3.032198	-2.905982
6	-7.062865	1.880238	-3.750637
6	-7.024048	-1.040817	4.028371
6	-6.866983	0.376636	4.188149
6	-6.812690	-0.939530	-4.069401
6	-6.690490	-2.254804	-3.497098
6	-6.558883	2.970184	3.049103
6	-6.414471	3.820969	1.895075
6	-6.432543	-3.920550	-1.198506
6	-6.300942	-4.084189	0.232248
6	-6.135669	4.122660	-0.925968
6	-6.007896	3.558392	-2.252886
6	-6.012916	-2.988468	2.849360
6	-5.860392	-1.845242	3.729620
6	-5.755357	1.313516	-3.993427
6	-5.633678	-0.120567	-4.194373
6	-5.549265	0.960769	4.117971
6	-5.397024	2.301058	3.572805
6	-5.386503	-2.749671	-3.125100
6	-5.259042	-3.633747	-1.979622
6	-5.103914	4.038568	1.333124
6	-4.964844	4.235523	-0.099192
6	-4.992204	-4.032605	0.834622
6	-4.849688	-3.510267	2.178729
6	-4.703508	3.189562	-2.743491
6	-4.578350	2.071797	-3.655454
6	-4.545785	-1.308956	3.971677
6	-4.389715	0.109957	4.205389
6	-4.328664	-0.733935	-4.123042
6	-4.204780	-2.080410	-3.617738
6	-4.079953	2.768233	3.208691
6	-3.932003	3.679664	2.099950
6	-3.948701	-3.888437	-1.420536
6	-3.815494	-4.131675	-0.005524
6	-3.651523	4.155770	-0.703977
6	-3.520526	3.666891	-2.054268
6	-3.528156	-3.176254	2.673861
6	-3.376320	-2.091105	3.611245
6	-3.265356	1.510427	-3.913847
6	-3.141324	0.099414	-4.190672
6	-3.063256	0.697409	4.154043
6	-2.908648	2.056300	3.689467
6	-2.892221	-2.592922	-3.269810
6	-2.765503	-3.542032	-2.185465
6	-2.611611	3.926291	1.550736
6	-2.472183	4.210952	0.137774
6	-2.499816	-4.110463	0.601419
6	-2.358187	-3.665306	1.974233
6	-2.209721	3.324137	-2.565013
6	-2.084289	2.255887	-3.539198
6	-2.057378	-1.569467	3.889928
6	-1.902032	-0.159899	4.205000
6	-1.836322	-0.518974	-4.161013
6	-1.713137	-1.900046	-3.730392
6	-1.592955	2.549008	3.359992

6	-1.444474	3.529732	2.299466
6	-1.460054	-3.833033	-1.644825
6	-1.328360	-4.161736	-0.238411
6	-1.164492	4.170048	-0.469138
6	-1.033434	3.759092	-1.852832
6	-1.045649	-3.360555	2.488506
6	-0.895527	-2.324778	3.488200
6	-0.779685	1.709062	-3.825599
6	-0.655591	0.312695	-4.178222
6	-0.584002	0.428322	4.182824
6	-0.428280	1.810275	3.793102
6	-0.406129	-2.426322	-3.406807
6	-0.279114	-3.433504	-2.381033
6	-0.127941	3.798999	1.763621
6	0.013412	4.164039	0.374981
6	-0.013410	-4.164568	0.369086
6	0.127943	-3.801494	1.758242
6	0.279115	3.436870	-2.376170
6	0.406128	2.431141	-3.403369
6	0.428279	-1.815643	3.790536
6	0.584000	-0.434243	4.182214
6	0.655589	-0.306782	-4.178662
6	0.779683	-1.703647	-3.828015
6	0.895527	2.319837	3.491488
6	1.045650	3.357028	2.493261
6	1.033436	-3.756466	-1.858152
6	1.164495	-4.169379	-0.475040
6	1.328362	4.162068	-0.232520
6	1.460055	3.835356	-1.639398
6	1.444475	-3.532984	2.294467
6	1.592955	-2.553762	3.356381
6	1.713135	1.905322	-3.727701
6	1.836319	0.524862	-4.160276
6	1.902030	0.153946	4.205225
6	2.057377	1.563958	3.892148
6	2.084288	-2.250876	-3.542390
6	2.209722	-3.320503	-2.569717
6	2.358189	3.662505	1.979419
6	2.499818	4.109603	0.607236
6	2.472186	-4.211141	0.131813
6	2.611613	-3.928480	1.545177
6	2.765503	3.545120	-2.180451
6	2.892220	2.597546	-3.266138
6	2.908647	-2.061521	3.686556
6	3.063254	-0.703289	4.153056
6	3.141321	-0.093483	-4.190812
6	3.265354	-1.504886	-3.915984
6	3.376319	2.085990	3.614204
6	3.528157	3.172463	2.678356
6	3.520528	-3.663977	-2.059457
6	3.651527	-4.154765	-0.709859
6	3.815496	4.131673	0.000324
6	3.948702	3.890440	-1.415032
6	3.932004	-3.682630	2.094741
6	4.079952	-2.772771	3.204772
6	4.204778	2.085528	-3.614795
6	4.328660	0.739770	-4.122005
6	4.389713	-0.115911	4.205235
6	4.545783	1.303331	3.973530
6	4.578349	-2.066620	-3.658387
6	4.703509	-3.185672	-2.748005
6	4.849689	3.507173	2.183696
6	4.992206	4.031411	0.840328
6	4.964847	-4.235369	-0.105186
6	5.103917	-4.040444	1.327407
6	5.259042	3.636541	-1.974479
6	5.386501	2.754090	-3.121209
6	5.397022	-2.306112	3.569551
6	5.549263	-0.966597	4.116616
6	5.633674	0.126504	-4.194206

6	5.755355	-1.307861	-3.995290
6	5.860390	1.839959	3.732233
6	6.012917	2.984425	2.853589
6	6.007899	-3.555191	-2.257921
6	6.135674	-4.121333	-0.931802
6	6.300944	4.083844	0.238027
6	6.432544	3.922234	-1.192957
6	6.414473	-3.823639	1.889667
6	6.558882	-2.974493	3.044902
6	6.690487	2.259752	-3.493911
6	6.812686	0.945291	-4.068079
6	6.866980	-0.382565	4.187624
6	7.024045	1.035112	4.029852
6	7.062863	-1.874924	-3.753303
6	7.188511	-3.028074	-2.910274
6	7.332561	3.329578	2.369354
6	7.476280	3.919131	1.071100
6	7.453979	-4.220204	-0.327851
6	7.597991	-4.124582	1.100302
6	7.749676	3.686163	-1.761959
6	7.883742	2.892612	-2.954514
6	7.892473	-2.531077	3.437268
6	8.044299	-1.232084	4.061652
6	8.135297	0.338605	-4.176459
6	8.257909	-1.101716	-4.057495
6	8.357430	1.584192	3.829182
6	8.512623	2.776380	3.016664
6	8.507123	-3.431248	-2.451281
6	8.626576	-4.075912	-1.157534
6	8.798993	4.018657	0.479419
6	8.923564	3.946077	-0.964116
6	8.921691	-4.002368	1.689443
6	9.054630	-3.220238	2.948937
6	9.200534	2.466805	-3.397646
6	9.311946	1.157158	-4.091726
6	9.354863	-0.668521	4.238750
6	9.512286	0.795919	4.159290
6	9.558032	-1.700457	-3.903792
6	9.684226	-2.923316	-3.098928
6	9.824634	3.185706	2.590194
6	9.970312	3.861286	1.296649
6	9.928163	-4.244474	-0.559950
6	10.044104	-4.264392	0.862863
6	10.225188	3.772275	-1.561571
6	10.333845	3.085116	-2.805906
6	10.328412	-2.793392	3.462862
6	10.473388	-1.566069	4.101253
6	10.578068	0.504486	-4.309577
6	10.696951	-0.876685	-4.233674
6	10.801888	1.431866	4.019923
6	10.951439	2.591568	3.276696
6	10.969345	-3.417366	-2.631624
6	11.088857	-4.068123	-1.421113
6	11.263454	4.042436	0.653392
6	11.388424	4.019746	-0.718936
1	-12.382853	-4.047453	-1.191145
1	-12.165902	-4.096590	1.270245
1	-12.081214	4.338288	-1.027050
1	-11.874215	3.179079	-3.199067
1	-11.960837	-2.985068	3.088180
1	-11.696284	-0.932879	4.405495
1	-11.696083	1.334313	-4.277484
1	-11.487478	-1.104606	-4.412702
1	-11.481406	1.213049	4.363895
1	-11.227200	3.376847	3.240817
1	-11.340684	-2.828237	-3.166445
1	-11.054515	4.237840	1.297313
1	11.054508	-4.239656	1.291315
1	11.340679	2.832714	-3.162455
1	11.227198	-3.381431	3.236055

1	11.481402	-1.219228	4.362202
1	11.487472	1.110859	-4.411161
1	11.696077	-1.328248	-4.279395
1	11.696281	0.926637	4.406830
1	11.960836	2.980679	3.092405
1	11.874219	-3.174517	-3.203562
1	12.081218	-4.336788	-1.033189
1	12.165905	4.094751	1.276038
1	12.382854	4.049103	-1.185422

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B3LYP/STO-3G Energy: -8371.757840

6	11.455711	-3.792368	1.707062
6	11.323035	-4.166113	0.387575
6	11.240437	4.208554	0.308523
6	11.120364	3.892435	1.645589
6	11.012115	-3.434646	-2.519448
6	10.870751	-2.503450	-3.535007
6	10.831390	1.851441	3.846561
6	10.699411	0.537895	4.275109
6	10.572896	0.376728	-4.382936
6	10.443520	1.728067	-4.081582
6	10.421861	-2.339669	3.485219
6	10.299376	-3.322397	2.460663
6	10.186523	3.821337	-1.946618
6	10.077094	4.169270	-0.566963
6	10.027868	-4.141319	-0.277594
6	9.882355	-3.819533	-1.700152
6	9.832310	3.548370	2.226932
6	9.698380	2.575262	3.318822
6	9.586588	-1.909653	-3.829928
6	9.444056	-0.513816	-4.282672
6	9.425287	-0.135303	4.235491
6	9.297440	-1.577648	3.901766
6	9.176064	2.286993	-3.691905
6	9.057107	3.367807	-2.675954
6	8.992599	-3.630180	1.931767
6	8.859387	-4.070436	0.555768
6	8.776571	4.174591	0.056754
6	8.657092	3.885629	1.473177
6	8.572362	-3.519057	-2.214634
6	8.425440	-2.573918	-3.306165
6	8.393329	2.050405	3.624896
6	8.257461	0.690261	4.110557
6	8.140336	0.091031	-4.254422
6	8.004918	1.508735	-3.984775
6	7.974520	-2.089002	3.586981
6	7.826046	-3.160878	2.638850
6	7.737901	3.652187	-2.135296
6	7.601672	4.113149	-0.779430
6	7.534831	-4.110967	-0.038364
6	7.390293	-3.873193	-1.443816
6	7.337021	3.627678	2.023169
6	7.204487	2.731824	3.134488
6	7.096976	-2.079563	-3.637845
6	6.953960	-0.749074	-4.154588
6	6.928441	0.090340	4.164866
6	6.790342	-1.325421	3.948546
6	6.677837	2.052814	-3.716387
6	6.547452	3.171050	-2.818280
6	6.503168	-3.520373	2.152742
6	6.361932	-4.042276	0.812371
6	6.284916	4.186453	-0.167323
6	6.157937	3.981625	1.259374
6	6.071044	-3.648627	-1.997243
6	5.925986	-2.767713	-3.140013
6	5.892163	2.260139	3.517460

6	5.757758	0.927182	4.079437
6	5.642038	-0.151561	-4.233899
6	5.506288	1.284767	-4.049898
6	5.479223	-1.885147	3.719672
6	5.336688	-3.031073	2.838468
6	5.241342	3.539830	-2.328044
6	5.111040	4.097270	-0.993133
6	5.050270	-4.131798	0.220182
6	4.905921	-3.968597	-1.212702
6	4.852252	3.764751	1.831092
6	4.721032	2.919125	2.999519
6	4.615854	-2.296843	-3.508938
6	4.473698	-0.983326	-4.098686
6	4.446920	0.330160	4.171708
6	4.307423	-1.099543	4.028410
6	4.196263	1.844481	-3.815376
6	4.062803	3.010375	-2.975582
6	4.021247	-3.405392	2.366413
6	3.877581	-3.999387	1.060578
6	3.800107	4.188127	-0.385149
6	3.670779	4.061686	1.045287
6	3.585522	-3.756321	-1.773202
6	3.440379	-2.946267	-2.956559
6	3.404008	2.456391	3.396008
6	3.268019	1.165749	4.026086
6	3.153897	-0.387225	-4.196712
6	3.015651	1.046013	-4.095693
6	2.987881	-1.669793	3.826695
6	2.845621	-2.861908	3.021338
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6	2.616999	4.038744	-1.210867
6	2.558044	-4.117682	0.471556
6	2.413396	-4.035935	-0.968050
6	2.358431	3.874247	1.629492
6	2.227678	3.093251	2.845072
6	2.124689	-2.498205	-3.356895
6	1.982870	-1.216295	-4.023729
6	1.956680	0.574566	4.160679
6	1.818028	-0.869404	4.099597
6	1.705991	1.621811	-3.901655
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6	1.390639	-3.940897	1.300393
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6	0.532550	0.810535	-4.130522
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6	-2.616999	4.038644	1.211203
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6	-7.826046	-3.160656	-2.639111
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6	-10.443519	1.727724	4.081718
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1	12.452266	-3.712544	2.163308
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6	0.810768	1.691673	3.862966
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6	1.104694	3.734765	1.889053
6	1.246055	4.140084	0.505772
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6	1.678207	-1.932763	3.761109
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6	1.898721	-0.197576	-4.179961
6	2.024311	-1.609200	-3.867159
6	2.125085	2.215765	3.580060
6	2.271717	3.281661	2.605745
6	2.283992	-3.707922	-1.949562
6	2.418155	-4.153053	-0.576279
6	2.556124	4.153957	-0.098629
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6	2.698628	-3.589056	2.210348
6	2.844032	-2.644870	3.296146
6	2.951618	1.994136	-3.655270
6	3.077971	0.634668	-4.127408
6	3.142209	0.039321	4.226678
6	3.291752	1.448345	3.954858
6	3.332369	-2.159555	-3.591769
6	3.462186	-3.246009	-2.652669
6	3.588770	3.600677	2.097850
6	3.732013	4.079291	0.746153
6	3.734368	-4.198754	0.029173
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6	4.006631	3.586441	-2.056646
6	4.136318	2.676193	-3.167257
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6	4.391035	0.018325	-4.182478
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6	4.615297	1.987552	3.700862
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6	4.778201	-3.605896	-2.158531
6	4.911621	-4.125269	-0.812840
6	5.049919	4.129254	0.143739
6	5.185657	3.918307	-1.283919
6	5.190117	-3.725317	2.000499
6	5.335198	-2.845154	3.146833
6	5.444728	2.179856	-3.533123
6	5.571225	0.844883	-4.090954
6	5.630313	-0.226150	4.230245
6	5.778112	1.207630	4.038721
6	5.823300	-1.968242	-3.718097
6	5.950778	-3.113283	-2.834183
6	6.074151	3.453017	2.309030
6	6.218045	4.009835	0.978495
6	6.220158	-4.200916	-0.211700
6	6.356909	-4.034106	1.218296
6	6.492681	3.666543	-1.839409
6	6.620359	2.817098	-3.000745
6	6.648142	-2.374495	3.518118
6	6.793913	-1.065186	4.098085
6	6.876400	0.231889	-4.174351
6	7.000947	-1.192558	-4.021359
6	7.094563	1.752799	3.802171
6	7.243892	2.904842	2.961429
6	7.262803	-3.484685	-2.350328
6	7.396566	-4.066872	-1.047547
6	7.535697	4.073106	0.379556
6	7.672326	3.940646	-1.040291
6	7.679284	-3.819034	1.784113
6	7.829692	-3.026471	2.975162
6	7.936913	2.331892	-3.384772
6	8.069565	1.051131	-4.026911
6	8.127105	-0.482910	4.211233
6	8.275102	0.955490	4.108201
6	8.325165	-1.772110	-3.822700
6	8.453245	-2.964146	-3.005634
6	8.573579	3.286002	2.508031
6	8.720074	3.918195	1.209674
6	8.718497	-4.188579	-0.456930
6	8.846769	-4.104787	0.985628
6	8.992016	3.736063	-1.610418
6	9.111967	2.955276	-2.827447
6	9.154775	-2.624833	3.417030
6	9.289799	-1.320990	4.120536
6	9.385459	0.462899	-4.205952
6	9.498731	-1.017398	-4.160051
6	9.583506	1.535231	3.973462
6	9.733264	2.766962	3.178440
6	9.756252	-3.405808	-2.581866
6	9.890558	-4.067380	-1.278385
6	10.028856	4.063630	0.628740
6	10.166965	4.007158	-0.828543
6	10.152350	-3.951289	1.579803
6	10.275432	-3.261325	2.822100
6	10.412698	2.508528	-3.265269
6	10.519768	1.295288	-4.003470
6	10.564970	-0.692540	4.347046
6	10.706730	0.689194	4.292311
6	10.767436	-1.691378	-4.033009
6	10.891609	-2.852598	-3.283958
6	11.020374	3.254160	2.735231
6	11.161731	3.892253	1.514596
6	11.180732	-4.264105	-0.634995
6	11.308711	-4.226817	0.737295
6	11.458021	3.847686	-1.484207

6	11.578378	3.145884	-2.663309
1	-12.570811	-2.942588	-3.088943
1	-12.361876	-4.206685	-0.975192
1	-12.303681	4.267910	1.201815
1	-12.081261	4.339039	-1.258190
1	-12.168268	-4.143191	1.156373
1	-11.917862	-3.011316	3.318744
1	-11.891803	3.268100	-3.106689
1	-11.673510	1.214572	-4.428962
1	-11.713850	-1.122557	4.342378
1	-11.465014	1.314463	4.437782
1	-11.526094	-0.900356	-4.193201
1	-11.287440	3.025805	3.175865
1	11.287448	-3.025749	3.175900
1	11.526088	0.900306	-4.193219
1	11.465014	-1.314405	4.437801
1	11.713849	1.122613	4.342369
1	11.673508	-1.214631	-4.428956
1	11.891803	-3.268140	-3.106653
1	11.917862	3.011357	3.318707
1	12.168268	4.143202	1.156321
1	12.081263	-4.339044	-1.258136
1	12.303684	-4.267882	1.201867
1	12.361877	4.206665	-0.975244
1	12.570811	2.942544	-3.088980

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B3LYP/STO-3G Energy: -8522.352500

6	-11.688356	-2.423901	-3.320418
6	-11.553435	-3.403003	-2.361549
6	-11.432107	3.829105	1.854105
6	-11.316177	4.218344	0.536925
6	-11.229730	-4.212818	0.523549
6	-11.080838	-3.908871	1.865657
6	-11.041499	3.537228	-2.387580
6	-10.916923	2.608851	-3.410462
6	-10.768268	-1.827922	4.027152
6	-10.634408	-0.505886	4.433625
6	-10.652124	-0.283379	-4.148657
6	-10.531525	-1.643763	-3.747077
6	-10.374606	2.369669	3.614346
6	-10.266591	3.355418	2.589970
6	-10.255231	-3.714676	-1.777450
6	-10.103611	-4.141711	-0.385229
6	-10.030027	4.203483	-0.144453
6	-9.902941	3.900334	-1.574330
6	-9.792082	-3.541345	2.409894
6	-9.642399	-2.554632	3.493232
6	-9.644928	1.999753	-3.714864
6	-9.523785	0.582166	-4.139551
6	-9.364652	0.170310	4.366345
6	-9.244237	1.611404	4.019299
6	-9.224174	-2.177934	-3.448163
6	-9.088896	-3.243584	-2.472724
6	-8.966954	3.667416	2.046348
6	-8.851622	4.119664	0.672723
6	-8.790364	-4.140602	0.204156
6	-8.635569	-3.861917	1.620420
6	-8.600990	3.593146	-2.106590
6	-8.473008	2.651892	-3.203512
6	-8.336347	-2.018538	3.763328
6	-8.196270	-0.653408	4.231188
6	-8.203363	-0.022144	-4.127070
6	-8.057924	-1.423659	-3.835618
6	-7.926020	2.124069	3.686204
6	-7.791070	3.196468	2.736869
6	-7.763295	-3.577095	-1.983598

6	-7.613022	-4.067763	-0.646402
6	-7.534364	4.164092	0.061529
6	-7.408225	3.936811	-1.347595
6	-7.304199	-3.598753	2.146620
6	-7.154001	-2.700346	3.253548
6	-7.147248	2.152624	-3.552863
6	-7.015957	0.816850	-4.067134
6	-6.867811	-0.050445	4.260935
6	-6.735491	1.364163	4.035332
6	-6.735059	-1.980862	-3.597970
6	-6.592214	-3.097987	-2.694592
6	-6.474803	3.560140	2.235749
6	-6.351293	4.088584	0.896099
6	-6.289809	-4.149591	-0.060671
6	-6.136731	-3.951527	1.366331
6	-6.097593	3.712043	-1.919524
6	-5.970900	2.833722	-3.068223
6	-5.837967	-2.223138	3.612413
6	-5.697279	-0.886093	4.164751
6	-5.706160	0.213010	-4.153374
6	-5.567494	-1.219349	-3.958136
6	-5.428408	1.925617	3.788511
6	-5.299053	3.071371	2.905401
6	-5.278731	-3.474295	-2.232126
6	-5.128746	-4.042810	-0.906985
6	-5.047315	4.180754	0.286739
6	-4.922207	4.024503	-1.148192
6	-4.823113	-3.728734	1.913862
6	-4.673632	-2.880625	3.077235
6	-4.663631	2.357213	-3.450968
6	-4.531667	1.044162	-4.037580
6	-4.386488	-0.286477	4.234398
6	-4.251283	1.142689	4.084011
6	-4.253625	-1.783122	-3.741610
6	-4.109141	-2.946694	-2.902665
6	-3.990036	3.448747	2.417293
6	-3.863808	4.045884	1.111345
6	-3.806041	-4.138144	-0.321571
6	-3.652788	-4.019951	1.106033
6	-3.608455	3.812942	-1.726704
6	-3.480128	3.004881	-2.913389
6	-3.351141	-2.413028	3.450524
6	-3.207940	-1.120796	4.074133
6	-3.214554	0.444255	-4.151306
6	-3.076745	-0.989245	-4.046198
6	-2.935228	1.714957	3.864062
6	-2.805403	2.906559	3.056752
6	-2.787604	-3.344971	-2.456060
6	-2.637236	-3.985152	-1.166672
6	-2.552064	4.166926	0.505322
6	-2.426545	4.088578	-0.936110
6	-2.331997	-3.830209	1.668642
6	-2.182414	-3.048705	2.881644
6	-2.170551	2.553454	-3.329460
6	-2.039831	1.271061	-3.995828
6	-1.895605	-0.526919	4.187620
6	-1.760166	0.916784	4.122695
6	-1.765415	-1.567072	-3.870913
6	-1.621855	-2.786011	-3.097314
6	-1.499825	3.314709	2.596026
6	-1.373844	3.989566	1.318561
6	-1.321639	-4.117023	-0.589019
6	-1.169152	-4.076553	0.851197
6	-1.120997	3.909299	-1.525072
6	-0.993797	3.164225	-2.758831
6	-0.868716	-2.603784	3.279526
6	-0.724899	-1.345648	3.976877
6	-0.730549	0.679159	-4.141162
6	-0.593403	-0.757831	-4.119721
6	-0.450529	1.496815	3.932042

6	-0.319524	2.730778	3.195602
6	-0.304099	-3.201425	-2.668050
6	-0.153408	-3.908992	-1.420829
6	-0.063356	4.131875	0.718305
6	0.063361	4.131924	-0.718029
6	0.153401	-3.909091	1.420562
6	0.304094	-3.201610	2.667831
6	0.319528	2.730995	-3.195421
6	0.450533	1.497082	-3.931944
6	0.593403	-0.758116	4.119667
6	0.730549	0.678872	4.141205
6	0.724898	-1.345379	-3.976969
6	0.868713	-2.603563	-3.279704
6	0.993800	3.164031	2.759041
6	1.121001	3.909189	1.525333
6	1.169146	-4.076501	-0.851476
6	1.321632	-4.117072	0.588737
6	1.373848	3.989650	-1.318294
6	1.499829	3.314880	-2.595806
6	1.621852	-2.786232	3.097123
6	1.765413	-1.567346	3.870805
6	1.760168	0.917057	-4.122636
6	1.895606	-0.526643	-4.187658
6	2.039833	1.270778	3.995909
6	2.170553	2.553215	3.329629
6	2.182411	-3.048519	-2.881852
6	2.331993	-3.830108	-1.668903
6	2.426549	4.088503	0.936383
6	2.552067	4.166950	-0.505043
6	2.637231	-3.985248	1.166400
6	2.787600	-3.345155	2.455832
6	2.805406	2.906755	-3.056559
6	2.935231	1.715208	-3.863949
6	3.076744	-0.989537	4.046128
6	3.214554	0.443956	4.151332
6	3.207940	-1.120532	-4.074209
6	3.351141	-2.412808	-3.450688
6	3.480130	3.004665	2.913588
6	3.608455	3.812808	1.726958
6	3.652785	-4.019894	-1.106308
6	3.806038	-4.138187	0.321289
6	3.863809	4.045944	-1.111074
6	3.990037	3.448897	-2.417062
6	4.109139	-2.946914	2.902464
6	4.253624	-1.783397	3.741486
6	4.251286	1.142951	-4.083934
6	4.386491	-0.286205	-4.234416
6	4.531667	1.043867	4.037645
6	4.663629	2.356958	3.451122
6	4.673632	-2.880434	-3.077430
6	4.823113	-3.728624	-1.914116
6	4.922205	4.024405	1.148461
6	5.047314	4.180755	-0.286458
6	5.128746	-4.042898	0.906710
6	5.278731	-3.474472	2.231891
6	5.299054	3.071553	-2.905195
6	5.428410	1.925859	-3.788383
6	5.567494	-1.219640	3.958050
6	5.706159	0.212707	4.153382
6	5.697282	-0.885826	-4.164810
6	5.837970	-2.222911	-3.612563
6	5.970897	2.833492	3.068409
6	6.097588	3.711892	1.919772
6	6.136733	-3.951459	-1.366600
6	6.289811	-4.149624	0.060390
6	6.351289	4.088628	-0.895823
6	6.474800	3.560276	-2.235509
6	6.592216	-3.098196	2.694383
6	6.735061	-1.981128	3.597835
6	6.735494	1.364423	-4.035238

6	6.867814	-0.050171	-4.260937
6	7.015955	0.816555	4.067182
6	7.147244	2.152364	3.553002
6	7.154005	-2.700142	-3.253730
6	7.304203	-3.598629	-2.146865
6	7.408217	3.936703	1.347859
6	7.534356	4.164080	-0.061247
6	7.613027	-4.067836	0.646127
6	7.763300	-3.577256	1.983359
6	7.791066	3.196643	-2.736651
6	7.926021	2.124309	-3.686056
6	8.057925	-1.423936	3.835521
6	8.203362	-0.022438	4.127063
6	8.196274	-0.653129	-4.231225
6	8.336351	-2.018291	-3.763460
6	8.473001	2.651665	3.203688
6	8.600981	3.592996	2.106832
6	8.635577	-3.861825	-1.620681
6	8.790373	-4.140610	-0.204436
6	8.851611	4.119704	-0.672443
6	8.966946	3.667552	-2.046098
6	9.088902	-3.243769	2.472509
6	9.224178	-2.178180	3.448016
6	9.244241	1.611679	-4.019180
6	9.364655	0.170605	-4.366319
6	9.523781	0.581883	4.139587
6	9.644922	1.999504	3.715001
6	9.642407	-2.554392	-3.493395
6	9.792090	-3.541179	-2.410127
6	9.902928	3.900239	1.574598
6	10.030014	4.203491	0.144739
6	10.103622	-4.141736	0.384951
6	10.255241	-3.714796	1.777198
6	10.266583	3.355616	-2.589743
6	10.374609	2.369921	-3.614170
6	10.531527	-1.644011	3.746960
6	10.652120	-0.283655	4.148640
6	10.634413	-0.505569	-4.433622
6	10.768277	-1.827632	-4.027245
6	10.916913	2.608657	3.410660
6	11.041486	3.537102	2.387837
6	11.080852	-3.908691	-1.865907
6	11.229748	-4.212725	-0.523822
6	11.316157	4.218453	-0.536647
6	11.432088	3.829307	-1.853858
6	11.553448	-3.403128	2.361296
6	11.688366	-2.424092	3.320230
1	-12.685662	-2.126535	-3.673489
1	-12.450414	-3.888414	-1.955652
1	-12.423251	3.742312	2.320891
1	-12.222312	4.444478	-0.039943
1	-12.238099	-4.372044	0.119970
1	-11.974078	-3.832281	2.499081
1	-12.042599	3.885906	-2.102553
1	-11.823246	2.243252	-3.910412
1	-11.772281	-2.268482	3.971779
1	-11.537008	0.064483	4.688663
1	-11.662278	0.139449	-4.223789
1	-11.381806	2.043142	3.903415
1	11.381839	2.043402	-3.903240
1	11.662262	0.139178	4.223812
1	11.537009	0.064841	-4.688591
1	11.772299	-2.268171	-3.971883
1	11.823236	2.243067	3.910613
1	12.042581	3.885829	2.102836
1	11.974098	-3.831992	-2.499313
1	12.238139	-4.371899	-0.120239
1	12.222282	4.444614	0.040225
1	12.423222	3.742614	-2.320663
1	12.450440	-3.888468	1.955337

1 12.685676 -2.126708 3.673295

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B3LYP/STO-3G Energy: -8597.649434

6	-11.767305	-1.442019	-3.903883
6	-11.645465	-2.634537	-3.226667
6	-11.543601	3.269934	2.696616
6	-11.413136	3.983656	1.525015
6	-11.352888	-4.161212	-0.643829
6	-11.216096	-4.213234	0.732134
6	-11.110028	4.077216	-1.473970
6	-10.977701	3.441873	-2.699202
6	-10.917754	-2.758281	3.357788
6	-10.783862	-1.585224	4.089691
6	-10.714979	0.832578	-4.148609
6	-10.603231	-0.585196	-4.106567
6	-10.507745	1.402742	4.033689
6	-10.386682	2.616662	3.297134
6	-10.353833	-3.093409	-2.730555
6	-10.217394	-3.864455	-1.494388
6	-10.119617	4.137540	0.874343
6	-9.978574	4.211807	-0.583385
6	-9.930951	-4.004650	1.363708
6	-9.788610	-3.330008	2.664500
6	-9.704009	2.922886	-3.137453
6	-9.583170	1.660790	-3.908943
6	-9.510957	-0.920742	4.208128
6	-9.383024	0.559997	4.241945
6	-9.300510	-1.186118	-3.943233
6	-9.178847	-2.466953	-3.272329
6	-9.080474	3.051283	2.864040
6	-8.949897	3.840702	1.653762
6	-8.909828	-4.023263	-0.913407
6	-8.767904	-4.118853	0.528344
6	-8.672052	4.044865	-1.164838
6	-8.535515	3.415714	-2.465526
6	-8.483576	-2.888311	3.074431
6	-8.343904	-1.688912	3.877341
6	-8.265367	1.065493	-4.039599
6	-8.127950	-0.364995	-4.114745
6	-8.060495	1.133947	4.063228
6	-7.913229	2.413035	3.421457
6	-7.859653	-2.922820	-2.873927
6	-7.724350	-3.741178	-1.706431
6	-7.626612	4.033568	1.086619
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6	-7.441090	-4.006615	1.115822
6	-7.298655	-3.422751	2.416851
6	-7.207940	3.014024	-2.918293
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6	-7.014023	-1.120415	4.071078
6	-6.875399	0.303392	4.216182
6	-6.809348	-0.972322	-4.015515
6	-6.679627	-2.283857	-3.427951
6	-6.590707	2.886092	3.042250
6	-6.452099	3.739697	1.885013
6	-6.406858	-3.978344	-1.149766
6	-6.266909	-4.153855	0.280741
6	-6.170151	4.096767	-0.930531
6	-6.033926	3.541578	-2.264042
6	-5.984005	-3.060126	2.897058
6	-5.844458	-1.910201	3.774082
6	-5.766454	1.284416	-3.981390
6	-5.634925	-0.150655	-4.158466
6	-5.563904	0.902546	4.133490
6	-5.422830	2.235897	3.575386
6	-5.371850	-2.774772	-3.066787

6	-5.237125	-3.665483	-1.930883
6	-5.141636	3.979129	1.332016
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6	-4.957817	-4.086813	0.878456
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6	-4.590512	2.051150	-3.646022
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6	-3.355094	-2.126682	3.646884
6	-3.274250	1.491965	-3.896296
6	-3.142645	0.079531	-4.161149
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6	1.834547	0.531377	-4.128738
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6	2.649035	-3.896735	1.563367
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6	9.704006	-2.923529	-3.136866
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B3LYP/STO-3G Energy: -8672.946093

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6	2.561181	-4.161158	0.453089
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6	3.013173	-1.691981	3.789866
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6	5.358882	-3.054538	2.786987
6	5.504897	-1.902031	3.654439
6	5.491253	1.237304	-4.050233
6	5.625546	-0.194918	-4.248188
6	5.779890	0.913614	4.032465
6	5.910747	2.254477	3.491947
6	5.908660	-2.822075	-3.181768
6	6.057158	-3.708813	-2.041246
6	6.163243	3.995110	1.250889
6	6.286714	4.189407	-0.180860
6	6.366617	-4.096329	0.765182
6	6.520833	-3.560331	2.100675
6	6.539669	3.120987	-2.813241
6	6.665585	1.999021	-3.713305
6	6.816670	-1.338463	3.864765
6	6.952876	0.078859	4.094484
6	6.936427	-0.799526	-4.187334
6	7.076016	-2.138147	-3.683318
6	7.218622	2.743007	3.115218
6	7.343739	3.648727	2.007805
6	7.377179	-3.940127	-1.496858
6	7.532740	-4.171436	-0.091507
6	7.597447	4.107040	-0.792125
6	7.722839	3.606302	-2.128276
6	7.844277	-3.192142	2.565512
6	7.991263	-2.102230	3.482672
6	7.983983	1.440314	-3.971950
6	8.123667	0.038800	-4.265398
6	8.272965	0.687382	4.022946
6	8.410574	2.050293	3.581664
6	8.407540	-2.642459	-3.363890
6	8.555194	-3.596033	-2.281189
6	8.666856	3.916807	1.454672
6	8.790886	4.190802	0.034701
6	8.865089	-4.133159	0.492358
6	9.021416	-3.671509	1.860145
6	9.039753	3.270001	-2.639804
6	9.157181	2.196202	-3.608450
6	9.314223	-1.563425	3.738518
6	9.443135	-0.153726	4.057114
6	9.443627	-0.566081	-4.303430
6	9.571278	-1.988212	-3.891792
6	9.727171	2.587689	3.289739
6	9.841511	3.608234	2.219166
6	9.864265	-3.920793	-1.783971
6	10.019688	-4.239247	-0.355763
6	10.091699	4.197693	-0.582679
6	10.217765	3.752172	-1.973266
6	10.334862	-3.372122	2.368159
6	10.483695	-2.311226	3.363776
6	10.458860	1.660433	-3.927877
6	10.571595	0.298476	-4.329225
6	10.748074	0.465042	4.048143
6	10.861289	1.844952	3.723620
6	10.845702	-2.603853	-3.619203
6	10.986829	-3.549527	-2.612283
6	11.111722	3.992946	1.650148
6	11.232346	4.292114	0.302214
6	11.311593	-4.282471	0.295952

6	11.462160	-3.880183	1.610825
6	11.504799	3.432700	-2.575836
6	11.622636	2.442545	-3.526463
6	11.780749	-1.744531	3.714302
6	11.909860	-0.419059	4.061957
1	-12.905021	0.018738	-4.220554
1	-12.680114	-2.363889	-3.601103
1	-12.613770	2.140853	3.892082
1	-12.409317	3.920490	2.189532
1	-12.470789	-3.815235	-2.038113
1	-12.203798	-4.527732	0.294932
1	-12.231183	4.460842	0.119785
1	-12.018886	3.929713	-2.265346
1	-11.992523	-3.902223	2.350422
1	-11.744458	-2.231483	4.128111
1	-11.868872	2.255021	-3.577905
1	-11.579881	-0.124297	4.421802
1	11.579885	-0.124653	-4.421812
1	11.868874	2.255301	3.577748
1	11.744455	-2.231810	-4.127956
1	11.992524	-3.902392	-2.350120
1	12.018891	3.929860	2.265032
1	12.231190	4.460789	-0.120142
1	12.203804	-4.527713	-0.294575
1	12.470790	-3.815044	2.038416
1	12.409319	3.920292	-2.189849
1	12.613766	2.140538	-3.892276
1	12.680110	-2.363604	3.601326
1	12.905016	0.019069	4.220602

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B3LYP/STO-3G Energy: -8748.242516

6	11.972022	-4.128440	0.626392
6	11.843679	-4.124739	-0.743660
6	11.766581	3.945772	1.473665
6	11.641819	3.276209	2.670820
6	11.542678	-2.621782	-3.339518
6	11.404733	-1.449676	-4.060243
6	11.343400	0.710519	4.228418
6	11.208711	-0.667476	4.280644
6	11.109949	1.552863	-4.089591
6	10.980288	2.768014	-3.431176
6	10.931979	-3.216308	2.730168
6	10.812212	-3.878111	1.477949
6	10.718543	4.192345	-0.803606
6	10.604744	4.148403	0.614831
6	10.548872	-3.913264	-1.381201
6	10.408285	-3.215365	-2.657818
6	10.349391	2.785823	3.131303
6	10.210873	1.554655	3.912977
6	10.119038	-0.795047	-4.184532
6	9.978358	0.668033	-4.238799
6	9.931358	-1.302621	4.052897
6	9.803636	-2.595578	3.338142
6	9.709188	3.200474	-2.905344
6	9.588125	3.959914	-1.634428
6	9.505590	-4.029491	0.880788
6	9.376931	-4.075590	-0.563697
6	9.300963	3.987307	1.213520
6	9.176631	3.321623	2.496717
6	9.099329	-2.786044	-3.077037
6	8.956088	-1.577483	-3.869217
6	8.903940	0.969072	4.063178
6	8.765245	-0.472841	4.158000
6	8.674758	1.244636	-4.052705
6	8.539337	2.535562	-3.405333
6	8.483186	-3.000756	2.892091

6	8.337892	-3.771415	1.685202
6	8.269412	4.089004	-1.040103
6	8.129847	4.159949	0.390145
6	8.055828	-3.949777	-1.150289
6	7.916201	-3.335458	-2.436211
6	7.855855	2.924614	2.950821
6	7.718737	1.759811	3.772701
6	7.629863	-1.008840	-4.055080
6	7.488755	0.410473	-4.187339
6	7.436221	-1.062227	4.038393
6	7.297680	-2.361091	3.443136
6	7.212057	2.985179	-2.998809
6	7.079684	3.812452	-1.831905
6	7.015661	-3.979899	1.113558
6	6.878660	-4.113905	-0.315166
6	6.809985	4.062875	0.995491
6	6.677839	3.476652	2.307594
6	6.596502	-2.964576	-2.910536
6	6.454956	-1.807103	-3.766395
6	6.401781	1.202502	4.006925
6	6.263692	-0.229723	4.181641
6	6.174108	1.009082	-4.102728
6	6.038185	2.337880	-3.534388
6	5.984402	-2.835940	3.065556
6	5.844730	-3.696497	1.905375
6	5.770145	4.036901	-1.262757
6	5.636811	4.208323	0.172735
6	5.567463	-4.038968	-0.914409
6	5.428197	-3.489348	-2.248725
6	5.369083	3.116187	2.796549
6	5.233141	1.982063	3.688587
6	5.145602	-1.252516	-3.998750
6	5.005581	0.173815	-4.206313
6	4.952779	-0.827536	4.104810
6	4.813041	-2.164465	3.574396
6	4.729022	2.815178	-3.160326
6	4.594493	3.707908	-2.033130
6	4.532558	-3.926700	1.344870
6	4.393745	-4.140592	-0.074667
6	4.326189	4.132311	0.779141
6	4.192432	3.618637	2.119361
6	4.111539	-3.129677	-2.733446
6	3.970165	-2.026182	-3.648028
6	3.915836	1.429600	3.936906
6	3.776013	0.018247	4.186769
6	3.687121	0.775421	-4.137313
6	3.548801	2.123104	-3.648421
6	3.493941	-2.653821	3.216524
6	3.353911	-3.577661	2.118673
6	3.277335	3.956107	-1.473954
6	3.143947	4.214352	-0.060753
6	3.074801	-4.089330	-0.678552
6	2.934938	-3.618036	-2.036990
6	2.875710	3.278774	2.625718
6	2.739404	2.197466	3.576601
6	2.652730	-1.482709	-3.912683
6	2.512453	-0.070566	-4.200947
6	2.460250	-0.585648	4.148740
6	2.320405	-1.954792	3.695201
6	2.235634	2.626317	-3.307178
6	2.100896	3.588294	-2.230414
6	2.040912	-3.846698	1.576281
6	1.902386	-4.147619	0.164509
6	1.834628	4.180899	0.549254
6	1.701934	3.745147	1.926197
6	1.623256	-3.291963	-2.544868
6	1.483114	-2.234640	-3.526157
6	1.429134	1.661969	3.859313
6	1.290181	0.258367	4.187002
6	1.202036	0.532617	-4.168903

6	1.063402	1.911427	-3.752761
6	1.009022	-2.462046	3.367685
6	0.868814	-3.449813	2.322176
6	0.791365	3.864550	-1.687298
6	0.657935	4.204895	-0.290404
6	0.589187	-4.123653	-0.439604
6	0.449439	-3.731028	-1.820598
6	0.389643	3.426740	2.445462
6	0.253194	2.403116	3.451187
6	0.167283	-1.703075	-3.813051
6	0.026358	-0.316033	-4.176953
6	-0.026365	-0.346471	4.174546
6	-0.167290	-1.730826	3.800548
6	-0.253197	2.428211	-3.433584
6	-0.389642	3.444480	-2.420428
6	-0.449438	-3.744204	1.793367
6	-0.589183	-4.126750	0.409548
6	-0.657929	4.202672	0.321041
6	-0.791363	3.852150	1.715416
6	-0.868814	-3.432795	-2.347247
6	-1.009025	-2.437433	-3.385527
6	-1.063408	1.884020	3.766586
6	-1.202044	0.502215	4.172670
6	-1.290188	0.288881	-4.185002
6	-1.429140	1.690059	-3.847096
6	-1.483119	-2.260289	3.509786
6	-1.623256	-3.310436	2.520821
6	-1.701931	3.759100	-1.898854
6	-1.834622	4.184801	-0.518770
6	-1.902382	-4.146322	-0.194724
6	-2.040910	-3.835112	-1.604265
6	-2.100894	3.571947	2.256505
6	-2.235637	2.602142	3.326224
6	-2.320409	-1.927804	-3.709334
6	-2.460256	-0.555391	-4.152880
6	-2.512462	-0.101185	4.200314
6	-2.652736	-1.511193	3.901771
6	-2.739406	2.223487	-3.560489
6	-2.875707	3.297841	-2.601754
6	-2.934936	-3.632805	2.010577
6	-3.074796	-4.094186	0.648738
6	-3.143940	4.213814	0.091465
6	-3.277330	3.945269	1.502746
6	-3.353909	-3.562131	-2.144683
6	-3.493943	-2.630306	-3.235764
6	-3.548805	2.096454	3.663783
6	-3.687129	0.745241	4.142836
6	-3.776018	0.048765	-4.186501
6	-3.915838	1.458263	-3.926367
6	-3.970170	-2.052728	3.633160
6	-4.111539	-3.149534	2.710569
6	-4.192426	3.634010	-2.092933
6	-4.326180	4.137905	-0.749005
6	-4.393739	-4.141046	0.044495
6	-4.532553	-3.916809	-1.373444
6	-4.594489	3.693002	2.060096
6	-4.729025	2.792071	3.180745
6	-4.813042	-2.138353	-3.590053
6	-4.952783	-0.797590	-4.110703
6	-5.005590	0.143150	4.207438
6	-5.145607	-1.281632	3.989498
6	-5.233141	2.008905	-3.674027
6	-5.369079	3.136506	-2.773760
6	-5.428195	-3.505668	2.223239
6	-5.567458	-4.045555	0.884953
6	-5.636802	4.209497	-0.142064
6	-5.770138	4.027618	1.292140
6	-5.844725	-3.682526	-1.932255
6	-5.984401	-2.813526	-3.086124
6	-6.038190	2.312058	3.551306

6	-6.174116	0.979149	4.109940
6	-6.263695	-0.199236	-4.183161
6	-6.401782	1.231681	-3.998029
6	-6.454961	-1.834514	3.753107
6	-6.596502	-2.985730	2.888851
6	-6.677832	3.493405	-2.282195
6	-6.809976	4.070063	-0.965858
6	-6.878654	-4.116120	0.285182
6	-7.015655	-3.971706	-1.142527
6	-7.079680	3.799025	1.859631
6	-7.212059	2.963253	3.020463
6	-7.297680	-2.335935	-3.460223
6	-7.436224	-1.032761	-4.045986
6	-7.488765	0.379941	4.190171
6	-7.629870	-1.038372	4.047591
6	-7.718737	1.787271	-3.759748
6	-7.855851	2.946065	-2.929420
6	-7.916200	-3.353150	2.411838
6	-8.055822	-3.958090	1.121479
6	-8.129838	4.162731	-0.359825
6	-8.269405	4.081357	1.069866
6	-8.337887	-3.759061	-1.712633
6	-8.483185	-2.979611	-2.913866
6	-8.539343	2.510680	3.423684
6	-8.674767	1.215063	4.061618
6	-8.765249	-0.442520	-4.161285
6	-8.903942	0.998667	-4.055969
6	-8.956096	-1.605648	3.857589
6	-9.099333	-2.808418	3.056641
6	-9.176625	3.339768	-2.472443
6	-9.300954	3.996104	-1.184439
6	-9.376924	-4.079634	0.533984
6	-9.505584	-4.022998	-0.910125
6	-9.588122	3.947938	1.663226
6	-9.709190	3.179229	2.928559
6	-9.803636	-2.571193	-3.356949
6	-9.931362	-1.273044	-4.062237
6	-9.978369	0.637119	4.243497
6	-10.119049	-0.825528	4.178580
6	-10.210874	1.583143	-3.901507
6	-10.349386	2.808601	-3.110909
6	-10.408286	-3.234685	2.634309
6	-10.548867	-3.923281	1.352649
6	-10.604736	4.152846	-0.584596
6	-10.718539	4.186427	0.834123
6	-10.812206	-3.867282	-1.506165
6	-10.931974	-3.196364	-2.753527
6	-10.980293	2.742938	3.451202
6	-11.109960	1.523013	4.100726
6	-11.208717	-0.636253	-4.285330
6	-11.343405	0.741326	-4.223066
6	-11.404743	-1.479236	4.049524
6	-11.542684	-2.646072	3.320297
6	-11.641811	3.295637	-2.646879
6	-11.766572	3.956477	-1.444889
6	-11.843672	-4.130122	0.713585
6	-11.972014	-4.123830	-0.656457
1	12.966245	-4.183636	1.091117
1	12.742575	-4.182621	-1.370982
1	12.760432	4.214816	1.089787
1	12.543484	3.017079	3.240699
1	12.546900	-3.029789	-3.167999
1	12.302279	-0.949215	-4.446054
1	12.346611	1.151851	4.285232
1	12.109365	-1.287729	4.376214
1	12.112199	1.200042	-4.364616
1	11.884320	3.346572	-3.200895
1	11.941794	-2.982690	3.091323
1	11.726931	4.165481	-1.236341
1	-11.726934	4.156388	1.266652

1	-11.941783	-2.960143	-3.112981
1	-11.884324	3.323159	3.225136
1	-12.112215	1.168189	4.373151
1	-12.109372	-1.255795	-4.385397
1	-12.346618	1.183060	-4.276650
1	-12.302292	-0.981593	4.438955
1	-12.546908	-3.052816	3.145804
1	-12.543475	3.040665	-3.218632
1	-12.760424	4.222726	-1.059068
1	-12.742565	-4.192583	1.340473
1	-12.966236	-4.175649	-1.121574

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B3LYP/STO-3G Energy: -8823.538697

6	12.109714	3.741688	-1.691373
6	11.987004	4.095889	-0.367668
6	11.829559	-4.276443	-0.420451
6	11.705004	-3.939621	-1.749802
6	11.684275	3.321599	2.529832
6	11.539722	2.377388	3.529189
6	11.422637	-1.861143	-3.917137
6	11.300228	-0.542483	-4.323091
6	11.220119	-0.513226	4.333126
6	11.077145	-1.855643	4.011933
6	11.052966	2.323554	-3.483514
6	10.944075	3.288615	-2.446477
6	10.790383	-3.911162	1.844866
6	10.669949	-4.236381	0.464774
6	10.692769	4.069047	0.305518
6	10.551646	3.728204	1.719081
6	10.414553	-3.571641	-2.318566
6	10.283571	-2.583941	-3.391438
6	10.248777	1.788309	3.820632
6	10.096225	0.390956	4.251195
6	10.029191	0.142778	-4.264452
6	9.916135	1.577223	-3.908381
6	9.799348	-2.397839	3.619234
6	9.665567	-3.459615	2.589783
6	9.641015	3.602915	-1.907064
6	9.518656	4.024480	-0.524197
6	9.364473	-4.223877	-0.152286
6	9.239868	-3.913215	-1.564038
6	9.240784	3.434589	2.238039
6	9.090945	2.473677	3.316566
6	8.981199	-2.044443	-3.685708
6	8.855204	-0.674640	-4.149943
6	8.786987	-0.202069	4.224325
6	8.637689	-1.615445	3.933459
6	8.601452	2.097327	-3.580779
6	8.467943	3.156183	-2.614787
6	8.343239	-3.726376	2.052694
6	8.196024	-4.165165	0.690253
6	8.199218	4.067644	0.077405
6	8.059778	3.809459	1.478884
6	7.920826	-3.634291	-2.102472
6	7.790475	-2.721041	-3.197752
6	7.761114	1.984559	3.645726
6	7.608887	0.649499	4.140984
6	7.532341	-0.061282	-4.184049
6	7.408009	1.348165	-3.945033
6	7.304901	-2.142446	3.660149
6	7.159721	-3.242011	2.748256
6	7.149906	3.518297	-2.114258
6	7.019758	4.019607	-0.769695
6	6.873975	-4.215113	0.083358
6	6.740607	-3.988334	-1.334862
6	6.738649	3.585814	2.035559

6	6.591163	2.691687	3.162039
6	6.477148	-2.230052	-3.565254
6	6.351302	-0.891422	-4.104539
6	6.288385	0.061524	4.217280
6	6.138627	-1.367159	4.013035
6	6.100227	1.917677	-3.701312
6	5.972854	3.050472	-2.803897
6	5.845035	-3.594261	2.260013
6	5.703016	-4.130702	0.918761
6	5.710049	4.115135	-0.169046
6	5.571628	3.931856	1.262378
6	5.432402	-3.754235	-1.897793
6	5.302669	-2.889173	-3.053345
6	5.278132	2.228676	3.533394
6	5.127411	0.906155	4.104270
6	5.046255	-0.281285	-4.183597
6	4.920945	1.148984	-4.017616
6	4.824009	-1.913161	3.779411
6	4.676315	-3.066249	2.922065
6	4.665258	3.430945	-2.320223
6	4.533952	4.006487	-1.004097
6	4.390406	-4.201699	0.316545
6	4.254650	-4.051703	-1.110878
6	4.254306	3.721993	1.826183
6	4.107800	2.895101	2.996055
6	3.989705	-2.406882	-3.433606
6	3.861842	-1.107612	-4.041055
6	3.804107	0.319423	4.196633
6	3.652361	-1.107082	4.074360
6	3.608132	1.727206	-3.796530
6	3.480591	2.904490	-2.975231
6	3.354458	-3.437775	2.449140
6	3.211473	-4.050882	1.151846
6	3.216885	4.124781	-0.405035
6	3.078405	4.022900	1.028603
6	2.938300	-3.840513	-1.684747
6	2.807463	-3.042599	-2.882815
6	2.786603	2.450656	3.395247
6	2.636190	1.164155	4.041066
6	2.551534	-0.501368	-4.158889
6	2.426072	0.939036	-4.076371
6	2.332936	-1.669624	3.879040
6	2.184539	-2.875630	3.088674
6	2.171665	3.317380	-2.518782
6	2.041078	3.973815	-1.232828
6	1.898651	-4.163261	0.557105
6	1.762872	-4.097497	-0.885073
6	1.765660	3.851577	1.606165
6	1.621123	3.086941	2.828993
6	1.500472	-2.586015	-3.292871
6	1.373347	-1.314992	-3.975103
6	1.320958	0.585634	4.171403
6	1.169230	-0.853069	4.128652
6	1.120763	1.527173	-3.890820
6	0.993473	2.753218	-3.135807
6	0.870324	-3.270861	2.639592
6	0.726326	-3.958405	1.377462
6	0.730269	4.118734	-0.640918
6	0.592672	4.097677	0.795133
6	0.451306	-3.910665	-1.465727
6	0.319773	-3.182438	-2.703184
6	0.302660	2.659869	3.246875
6	0.152478	1.417359	3.960507
6	0.063233	-0.714672	-4.119086
6	-0.063230	0.720528	-4.118068
6	-0.152476	-1.422989	3.958492
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6	-0.319773	3.186281	-2.698663
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6	-0.726330	3.956439	1.383082
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6	-0.993473	-2.748753	-3.139713
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6	-1.169228	0.847197	4.129860
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6	-1.500469	2.590696	-3.289200
6	-1.621122	-3.090962	2.824609
6	-1.765662	-3.853856	1.600694
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6	-2.171667	-3.313788	-2.523490
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6	-2.551529	0.507283	-4.158180
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6	-2.786600	-2.455484	3.391770
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6	-3.078407	-4.024355	1.022890
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6	-3.211478	4.049230	1.157595
6	-3.354463	3.434279	2.454017
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6	-3.861836	1.113361	-4.039490
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6	-4.665263	-3.427628	-2.325089
6	-4.676320	3.062077	2.926411
6	-4.824011	1.907776	3.782125
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6	-5.127406	-0.911996	4.102996
6	-5.278127	-2.233705	3.530242
6	-5.302664	2.893518	-3.049256
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6	-5.710053	-4.114875	-0.174885
6	-5.703023	4.129369	0.924618
6	-5.845043	3.591020	2.265105
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6	-6.100229	-1.912400	-3.704033
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6	-6.288381	-0.067529	4.217206
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6	-6.477141	2.235130	-3.562110
6	-6.591157	-2.696190	3.158235
6	-6.738646	-3.588706	2.030478
6	-6.740609	3.990220	-1.329210
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6	-7.532334	0.067242	-4.183982
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6	-8.059777	-3.811553	1.473488
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6	-8.196032	4.164142	0.696151
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6	-8.467950	-3.152427	-2.619252
6	-8.601455	-2.092208	-3.583750
6	-8.637690	1.609830	3.935756
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6	-8.855196	0.680556	-4.149021
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6	-9.239869	3.915427	-1.558504
6	-9.364480	4.224055	-0.146307
6	-9.518662	-4.023694	-0.529895
6	-9.641023	-3.600154	-1.912158
6	-9.665576	3.455883	2.594674
6	-9.799353	2.392659	3.622634
6	-9.916135	-1.571637	-3.910622
6	-10.029184	-0.136694	-4.264688
6	-10.096218	-0.397022	4.250679
6	-10.248768	-1.793763	3.818139
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6	-10.414550	3.574938	-2.313530
6	-10.551644	-3.730643	1.713814
6	-10.692772	-4.069445	0.299761
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6	-10.790392	3.908478	1.850394
6	-10.944083	-3.285076	-2.451119
6	-11.052970	-2.318553	-3.486795
6	-11.077147	1.849906	4.014577
6	-11.220115	0.507040	4.333889
6	-11.300219	0.548655	-4.322380
6	-11.422626	1.866739	-3.914562
6	-11.539713	-2.382434	3.525870
6	-11.684269	-3.325210	2.525159
6	-11.705004	3.942089	-1.744241
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6	-11.987011	-4.095304	-0.373455
6	-12.109723	-3.739206	-1.696652
1	13.102316	3.665517	-2.156580
1	12.888738	4.307638	0.221368
1	12.822618	-4.447724	0.017668
1	12.605914	-3.847608	-2.370139
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1	12.205749	0.023062	-4.578473
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1	11.974935	-2.482932	3.937741
1	12.059194	1.994543	-3.773721
1	11.801033	-3.783181	2.253772
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1	-12.059199	-1.989130	-3.776534
1	-11.974941	2.477294	3.941268
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1	-12.421297	2.318113	-3.857455
1	-12.434421	-1.992156	4.027961
1	-12.690891	-3.666508	2.252054
1	-12.605911	3.850967	-2.364713
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1	-13.102328	-3.662354	-2.161741

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6	12.197881	-3.256366	2.556400
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6	11.564961	2.735852	3.273419
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6	11.169902	0.693530	-4.386469
6	11.163014	-1.416196	3.928421
6	11.040381	-2.613633	3.174837
6	10.912120	3.239025	-2.818326
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6	10.765060	-4.073782	0.717377
6	10.617046	-4.107438	-0.734823
6	10.558875	3.985965	1.293129
6	10.427442	3.308959	2.583844
6	10.314691	-2.771067	-3.263431
6	10.170033	-1.530340	-4.037259
6	10.159076	0.900166	4.128911
6	10.033697	-0.575939	4.153165
6	9.898282	1.329828	-4.140544
6	9.778921	2.620958	-3.418032
6	9.731263	-3.045208	2.740494
6	9.596633	-3.807298	1.513339
6	9.500315	4.067749	-0.963875
6	9.381939	4.132183	0.480728
6	9.304774	-3.946189	-1.306230
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6	9.122993	2.874661	3.012726
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6	8.566296	-2.421931	3.315196
6	8.462217	3.028868	-2.962649
6	8.326538	3.804539	-1.758166
6	8.273242	-3.992409	0.949115
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6	7.681688	-1.729652	-3.853903
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6	7.527821	-0.323748	4.141117
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6	7.270856	2.392247	-3.505515
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6	6.072949	-2.249579	3.482474
6	5.961503	2.870065	-3.119108
6	5.831548	3.734063	-1.960493
6	5.784960	-3.953062	1.210813
6	5.638098	-4.142639	-0.218844
6	5.575101	4.096472	0.859206
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6	5.342190	-3.078426	-2.850127
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6	4.918468	0.864315	-4.152130
6	4.785007	2.200544	-3.619340
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6	4.170610	-3.573100	-2.154060
6	4.132375	3.201439	2.695576
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6	1.829864	-4.118262	-0.553720
6	1.682531	-3.691917	-1.931027
6	1.642656	3.358530	2.522648
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6	1.253219	-0.216693	-4.202490
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6	0.592409	4.177723	0.420398
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6	-1.239067	-0.457366	-4.164888
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6	-2.029665	3.891777	1.604895
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6	-2.268417	-2.549017	-3.294149
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6	-2.425004	0.625891	4.175766
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6	-2.684946	1.559158	-3.892784
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6	-2.849723	-3.233531	2.647484
6	-2.950749	3.683431	-2.003529
6	-3.080379	4.145275	-0.640887
6	-3.145968	-4.147551	-0.042531
6	-3.293802	-3.879946	-1.452845
6	-3.338522	3.618858	2.155936
6	-3.469247	2.692659	3.252582
6	-3.583586	-2.043219	-3.622568
6	-3.724557	-0.696003	-4.112636
6	-3.739121	0.019867	4.224789
6	-3.878927	-1.391074	3.976039
6	-3.999189	2.103867	-3.617430
6	-4.132375	3.201574	-2.695417
6	-4.170610	-3.573209	2.153877
6	-4.318857	-4.072890	0.811324
6	-4.395018	4.191665	-0.026901
6	-4.523444	3.969024	1.391856
6	-4.615670	-3.623741	-1.995644
6	-4.759928	-2.730612	-3.119432
6	-4.785005	2.200360	3.619449
6	-4.918466	0.864104	4.152173
6	-5.042430	-0.091438	-4.171863
6	-5.178577	1.332540	-3.963501
6	-5.197904	-1.946251	3.741609
6	-5.342189	-3.078570	2.849971
6	-5.446129	3.559046	-2.198796
6	-5.575102	4.096514	-0.859001
6	-5.638099	-4.142648	0.218633
6	-5.784962	-3.952998	-1.211014
6	-5.831547	3.733961	1.960680
6	-5.961502	2.869905	3.119252
6	-6.072951	-2.249402	-3.482590
6	-6.214091	-0.925541	-4.057937
6	-6.227269	0.264504	4.242107
6	-6.364750	-1.169221	4.072771
6	-6.487320	1.890574	-3.724065
6	-6.619329	3.043657	-2.858332
6	-6.654486	-3.442007	2.377599
6	-6.802847	-4.017123	1.060313
6	-6.881895	4.166560	-0.249457
6	-7.008529	4.019916	1.179219
6	-7.099678	-3.717263	-1.760964
6	-7.242467	-2.888838	-2.930333
6	-7.270854	2.392068	3.505636
6	-7.402051	1.094476	4.104925
6	-7.527823	-0.323538	-4.141135
6	-7.663529	1.098403	-4.009662
6	-7.681685	-1.729848	3.853820
6	-7.826949	-2.893903	3.032790
6	-7.934292	3.412880	-2.371737
6	-8.064477	4.012384	-1.077906
6	-8.126316	-4.102278	0.470746
6	-8.273243	-3.992357	-0.949315
6	-8.326537	3.804447	1.758358
6	-8.462216	3.028716	2.962802
6	-8.566298	-2.421761	-3.315317
6	-8.713548	-1.151436	-3.976546
6	-8.728834	0.503200	4.239488
6	-8.865441	-0.938943	4.158459
6	-8.990227	1.671287	-3.813893
6	-9.122995	2.874814	-3.012582
6	-9.154963	-3.294029	2.595028
6	-9.304774	-3.946251	1.306034
6	-9.381940	4.132205	-0.480518

6	-9.500315	4.067697	0.964081
6	-9.596636	-3.807217	-1.513528
6	-9.731266	-3.045066	-2.740645
6	-9.778920	2.620783	3.418167
6	-9.898280	1.329617	4.140617
6	-10.033699	-0.575727	-4.153195
6	-10.159077	0.900377	-4.128868
6	-10.170030	-1.530546	4.037192
6	-10.314689	-2.771233	3.263299
6	-10.427443	3.309090	-2.583676
6	-10.558876	3.986030	-1.292926
6	-10.617045	-4.107473	0.734621
6	-10.765061	-4.073742	-0.717579
6	-10.802351	3.909238	1.568785
6	-10.912118	3.238882	2.818494
6	-11.040383	-2.613469	-3.174966
6	-11.163016	-1.415994	-3.928489
6	-11.169899	0.693306	4.386517
6	-11.300617	-0.687405	4.353340
6	-11.435713	1.567247	-4.004587
6	-11.564963	2.736017	-3.273276
6	-11.603415	-3.277878	2.836198
6	-11.747550	-3.934133	1.628438
6	-11.848752	4.184940	-0.643254
6	-11.967717	4.166922	0.728162
6	-12.063825	-3.937876	-1.369446
6	-12.197884	-3.256227	-2.556557
1	13.194006	-3.072302	2.982347
1	12.959903	-4.302710	0.850654
1	12.959295	4.212273	-1.199567
1	12.752502	4.249216	1.263203
1	12.753343	-4.204267	-1.282005
1	12.497360	-3.038014	-3.426557
1	12.566388	3.150036	3.099314
1	12.338445	1.078730	4.394087
1	12.302625	-1.130071	-4.421743
1	12.072608	1.311061	-4.480213
1	12.173226	-1.032259	4.120429
1	11.919173	3.001588	-3.184939
1	-11.919163	3.001436	3.185099
1	-12.173234	-1.032042	-4.120471
1	-12.072605	1.310831	4.480295
1	-12.302614	-1.130296	4.421720
1	-12.338447	1.078953	-4.394030
1	-12.566393	3.150187	-3.099141
1	-12.497357	-3.038192	3.426415
1	-12.753336	-4.204344	1.281810
1	-12.752503	4.249276	-1.262985
1	-12.959298	4.212197	1.199783
1	-12.959905	-4.302656	-0.850863
1	-13.194011	-3.072134	-2.982488

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6	-12.299023	-2.428048	-3.359860
6	-12.177947	-3.391686	-2.386364
6	-12.056893	3.899239	1.714148
6	-11.926478	4.268220	0.394657
6	-11.884792	-4.161369	0.513834
6	-11.746514	-3.838744	1.850107
6	-11.628188	3.542669	-2.517649
6	-11.499053	2.599771	-3.522749
6	-11.442417	-1.726103	3.982250
6	-11.305285	-0.401131	4.367635
6	-11.243222	-0.305790	-4.208862
6	-11.133124	-1.656302	-3.785823
6	-11.022879	2.458601	3.503052

6	-10.899620	3.425651	2.468287
6	-10.884857	-3.699441	-1.782854
6	-10.748146	-4.106267	-0.388006
6	-10.631983	4.233680	-0.275898
6	-10.493184	3.910744	-1.695625
6	-10.458145	-3.467158	2.400800
6	-10.313210	-2.467906	3.467303
6	-10.224583	1.977124	-3.804714
6	-10.107027	0.556078	-4.204551
6	-10.028215	0.268569	4.300300
6	-9.896943	1.700016	3.932765
6	-9.829537	-2.194439	-3.468563
6	-9.708618	-3.246475	-2.477132
6	-9.591583	3.725611	1.933450
6	-9.460871	4.158431	0.554926
6	-9.439270	-4.107256	0.213718
6	-9.295853	-3.809354	1.627958
6	-9.187295	3.592275	-2.213211
6	-9.054192	2.633554	-3.295602
6	-9.006595	-1.936176	3.744552
6	-8.863610	-0.563614	4.192816
6	-8.791711	-0.055331	-4.173052
6	-8.656790	-1.453711	-3.857755
6	-8.575008	2.202382	3.606235
6	-8.425853	3.259939	2.641542
6	-8.390962	-3.580042	-1.971428
6	-8.255526	-4.051844	-0.626292
6	-8.139434	4.187088	-0.044400
6	-8.001430	3.938982	-1.447798
6	-7.969458	-3.543877	2.161766
6	-7.824617	-2.630327	3.254504
6	-7.729259	2.120004	-3.622359
6	-7.600224	0.778467	-4.112378
6	-7.533194	0.033541	4.221967
6	-7.391073	1.439783	3.975583
6	-7.338731	-2.013364	-3.596770
6	-7.209600	-3.114302	-2.678215
6	-7.102123	3.607627	2.145629
6	-6.962825	4.114734	0.803988
6	-6.935998	-4.129906	-0.026372
6	-6.794476	-3.913168	1.394541
6	-6.684015	3.696981	-2.003917
6	-6.550720	2.803963	-3.134863
6	-6.506140	-2.153067	3.617554
6	-6.362930	-0.812224	4.149274
6	-6.290117	0.165482	-4.177505
6	-6.160983	-1.262076	-3.959844
6	-6.075982	1.992134	3.733331
6	-5.932575	3.123137	2.836149
6	-5.900240	-3.493185	-2.199241
6	-5.765279	-4.044017	-0.865384
6	-5.651058	4.194830	0.205573
6	-5.513399	4.018000	-1.226279
6	-5.483703	-3.692263	1.952437
6	-5.340407	-2.827359	3.105525
6	-5.242870	2.316512	-3.500838
6	-5.112889	0.992421	-4.066599
6	-5.050715	-0.218419	4.224788
6	-4.906891	1.209144	4.053483
6	-4.853805	-1.830243	-3.724668
6	-4.723404	-2.982879	-2.866496
6	-4.619203	3.487904	2.355792
6	-4.477889	4.065745	1.042139
6	-4.450583	-4.138101	-0.266707
6	-4.309692	-3.999824	1.159963
6	-4.197718	3.790055	-1.788881
6	-4.062432	2.964178	-2.960355
6	-4.020789	-2.359341	3.481974
6	-3.876081	-1.060645	4.085079
6	-3.799231	0.383163	-4.155508

6	-3.669894	-1.045410	-4.027045
6	-3.586245	1.770322	3.833588
6	-3.442418	2.945383	3.012561
6	-3.407480	-3.379342	-2.399429
6	-3.271700	-3.999770	-1.104351
6	-3.158407	4.168549	0.445525
6	-3.019221	4.069605	-0.988065
6	-2.990506	-3.806090	1.731723
6	-2.847220	-3.010760	2.930290
6	-2.748421	2.497825	-3.356531
6	-2.618056	1.208961	-4.000505
6	-2.558213	-0.470918	4.201226
6	-2.414258	0.967536	4.116551
6	-2.359971	-1.628720	-3.831596
6	-2.229849	-2.835569	-3.041114
6	-2.127458	3.342533	2.559159
6	-1.986107	3.999302	1.274929
6	-1.959607	-4.133784	-0.512880
6	-1.819997	-4.074456	0.928244
6	-1.707838	3.878923	-1.563831
6	-1.573071	3.114548	-2.786614
6	-1.534473	-2.569501	3.336959
6	-1.390419	-1.299893	4.017687
6	-1.311350	0.608849	-4.128318
6	-1.182507	-0.830887	-4.084364
6	-1.101508	1.538754	3.932403
6	-0.957538	2.763189	3.178285
6	-0.920513	-3.253445	-2.595675
6	-0.785051	-3.944660	-1.335589
6	-0.672418	4.127781	0.685381
6	-0.532427	4.106293	-0.750083
6	-0.504763	-3.905324	1.507071
6	-0.361768	-3.180295	2.744245
6	-0.260888	2.666359	-3.202321
6	-0.129759	1.422151	-3.916611
6	-0.072410	-0.716277	4.160236
6	0.072411	0.716510	4.160196
6	0.129759	-1.422369	-3.916532
6	0.260888	-2.666537	-3.202173
6	0.361768	3.180450	2.744067
6	0.504763	3.905410	1.506854
6	0.532427	-4.106333	-0.749853
6	0.672418	-4.127741	0.685612
6	0.785052	3.944588	-1.335809
6	0.920513	3.253301	-2.595856
6	0.957538	-2.763011	3.178440
6	1.101508	-1.538534	3.932489
6	1.182507	0.830660	-4.084410
6	1.311349	-0.609078	-4.128284
6	1.390419	1.300118	4.017614
6	1.534473	2.569689	3.336816
6	1.573071	-3.114703	-2.786440
6	1.707838	-3.879009	-1.563615
6	1.819997	4.074510	0.928017
6	1.959608	4.133758	-0.513110
6	1.986106	-3.999230	1.275153
6	2.127457	-3.342389	2.559346
6	2.229850	2.835400	-3.041271
6	2.359971	1.628507	-3.831685
6	2.414258	-0.967306	4.116605
6	2.558213	0.471154	4.201200
6	2.618056	-1.209183	-4.000437
6	2.748421	-2.498011	-3.356391
6	2.847219	3.010926	2.930123
6	2.990506	3.806189	1.731512
6	3.019221	-4.069659	-0.987838
6	3.158407	-4.168524	0.445758
6	3.271701	3.999710	-1.104572
6	3.407481	3.379209	-2.399616
6	3.442418	-2.945214	3.012726

6	3.586245	-1.770108	3.833687
6	3.669895	1.045186	-4.027101
6	3.799230	-0.383394	-4.155486
6	3.876080	1.060874	4.085020
6	4.020789	2.359537	3.481843
6	4.062431	-2.964343	-2.960190
6	4.197717	-3.790154	-1.788670
6	4.309693	3.999890	1.159742
6	4.450584	4.138086	-0.266936
6	4.477889	-4.065686	1.042366
6	4.619204	-3.487771	2.355987
6	4.723405	2.982719	-2.866660
6	4.853806	1.830035	-3.724767
6	4.906890	-1.208917	4.053551
6	5.050715	0.218656	4.224777
6	5.112888	-0.992648	-4.066544
6	5.242869	-2.316707	-3.500709
6	5.340407	2.827534	3.105369
6	5.483703	3.692374	1.952234
6	5.513399	-4.018068	-1.226055
6	5.651058	-4.194816	0.205807
6	5.765280	4.043968	-0.865607
6	5.900242	3.493061	-2.199433
6	5.932575	-3.122978	2.836324
6	6.075981	-1.991925	3.733442
6	6.160983	1.261854	-3.959913
6	6.290116	-0.165715	-4.177496
6	6.362929	0.812458	4.149231
6	6.506140	2.153271	3.617435
6	6.550719	-2.804139	-3.134707
6	6.684015	-3.697093	-2.003712
6	6.794477	3.913246	1.394325
6	6.935999	4.129903	-0.026600
6	6.962825	-4.114687	0.804218
6	7.102123	-3.607505	2.145830
6	7.209602	3.114150	-2.678386
6	7.338731	2.013162	-3.596880
6	7.391072	-1.439559	3.975663
6	7.533193	-0.033304	4.221971
6	7.600222	-0.778699	-4.112337
6	7.729258	-2.120208	-3.622243
6	7.824617	2.630510	3.254360
6	7.969459	3.543998	2.161571
6	8.001429	-3.939062	-1.447580
6	8.139435	-4.187088	-0.044167
6	8.255527	4.051806	-0.626515
6	8.390964	3.579929	-1.971625
6	8.425853	-3.259790	2.641723
6	8.575008	-2.202179	3.606358
6	8.656790	1.453494	-3.857837
6	8.791708	0.055096	-4.173060
6	8.863610	0.563850	4.192788
6	9.006595	1.936385	3.744448
6	9.054190	-2.633741	-3.295459
6	9.187295	-3.592401	-2.213014
6	9.295854	3.809443	1.627748
6	9.439272	4.107266	0.213491
6	9.460872	-4.158395	0.555156
6	9.591583	-3.725501	1.933656
6	9.708620	3.246333	-2.477311
6	9.829536	2.194244	-3.468687
6	9.896942	-1.699796	3.932861
6	10.028214	-0.268328	4.300316
6	10.107025	-0.556316	-4.204525
6	10.224581	-1.977340	-3.804610
6	10.313211	2.468098	3.467167
6	10.458146	3.467290	2.400609
6	10.493184	-3.910837	-1.695410
6	10.631984	-4.233689	-0.275664
6	10.748148	4.106239	-0.388232

6	10.884859	3.699335	-1.783057
6	10.899620	-3.425510	2.468476
6	11.022879	-2.458405	3.503191
6	11.133122	1.656086	-3.785917
6	11.243218	0.305552	-4.208896
6	11.305284	0.401374	4.367616
6	11.442418	1.726322	3.982153
6	11.499050	-2.599974	-3.522612
6	11.628187	-3.542806	-2.517455
6	11.746514	3.838844	1.849896
6	11.884794	4.161390	0.513606
6	11.926477	-4.268191	0.394894
6	12.056892	-3.899140	1.714363
6	12.177950	3.391541	-2.386550
6	12.299023	2.427851	-3.359995
1	-13.290740	-2.134401	-3.731244
1	-13.079971	-3.871109	-1.984571
1	-13.052051	3.829493	2.175264
1	-12.824592	4.496711	-0.193656
1	-12.889126	-4.327550	0.103368
1	-12.643454	-3.753570	2.477120
1	-12.628536	3.906987	-2.250898
1	-12.400771	2.234955	-4.031494
1	-12.446778	-2.165671	3.930288
1	-12.205423	0.177925	4.611501
1	-12.249641	0.122020	-4.303779
1	-12.033940	2.142116	3.790768
1	12.033937	-2.141908	3.790890
1	12.249618	-0.122253	-4.303805
1	12.205423	-0.177670	4.611510
1	12.446783	2.165882	3.930155
1	12.400768	-2.235193	-4.031383
1	12.628544	-3.907099	-2.250673
1	12.643455	3.753707	2.476914
1	12.889133	4.327545	0.103131
1	12.824592	-4.496715	-0.193405
1	13.052053	-3.829372	2.175474
1	13.079975	3.870985	-1.984781
1	13.290737	2.134184	-3.731365

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6	12.425421	-1.530421	3.802500
6	12.293239	-2.710220	3.108957
6	12.158517	3.283452	-2.722664
6	12.040785	3.978488	-1.540806
6	11.972862	-4.194695	0.504613
6	11.823597	-4.225106	-0.868329
6	11.765413	4.025337	1.462216
6	11.641680	3.373596	2.676807
6	11.506573	-2.729602	-3.468711
6	11.369715	-1.547873	-4.180581
6	11.382840	0.743527	4.087619
6	11.265204	-0.669171	4.025376
6	11.103920	1.438809	-4.075422
6	10.992933	2.638547	-3.321797
6	10.993856	-3.155670	2.613809
6	10.843950	-3.904898	1.371312
6	10.751796	4.123747	-0.873770
6	10.624201	4.176378	0.581618
6	10.531051	-4.000982	-1.486026
6	10.379444	-3.308793	-2.771597
6	10.367252	2.851009	3.118894
6	10.248655	1.581492	3.870856
6	10.094814	-0.876673	-4.277343
6	9.971277	0.601235	-4.288073
6	9.957127	-1.264334	3.866671

6	9.824747	-2.534454	3.178627
6	9.690390	3.072856	-2.871746
6	9.573124	3.844955	-1.649121
6	9.529701	-4.054355	0.800117
6	9.374601	-4.128387	-0.642167
6	9.321660	4.009141	1.173713
6	9.194624	3.361228	2.467152
6	9.071827	-2.859951	-3.166410
6	8.928776	-1.647664	-3.951113
6	8.931511	0.989183	4.007370
6	8.789961	-0.442838	4.062079
6	8.654145	1.177599	-4.091131
6	8.517095	2.447877	-3.428203
6	8.502149	-2.979984	2.785423
6	8.353775	-3.779880	1.607014
6	8.257338	4.033527	-1.067191
6	8.130597	4.154135	0.353927
6	8.044558	-4.002134	-1.215885
6	7.892465	-3.398786	-2.505132
6	7.871119	2.955331	2.924407
6	7.742022	1.785392	3.742978
6	7.600122	-1.070899	-4.121468
6	7.464579	0.351830	-4.242782
6	7.468153	-1.044032	3.962626
6	7.328112	-2.342425	3.358160
6	7.198994	2.917917	-3.027454
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6	7.028696	-4.002385	1.057102
6	6.875137	-4.156255	-0.370041
6	6.816955	4.069548	0.963439
6	6.690155	3.497382	2.285915
6	6.571690	-3.023526	-2.967908
6	6.427480	-1.863851	-3.824306
6	6.430238	1.216033	3.972663
6	6.295125	-0.218455	4.129663
6	6.153060	0.954916	-4.139876
6	6.021420	2.278646	-3.562107
6	6.013328	-2.825371	3.002557
6	5.865351	-3.699094	1.855798
6	5.766583	3.990677	-1.292250
6	5.640540	4.187399	0.137984
6	5.559792	-4.079764	-0.955805
6	5.408390	-3.538535	-2.290949
6	5.383787	3.127080	2.774558
6	5.254432	1.992909	3.662093
6	5.116304	-1.302486	-4.039487
6	4.978585	0.122209	-4.239429
6	4.984585	-0.821499	4.058282
6	4.843887	-2.155486	3.525813
6	4.713847	2.761955	-3.181814
6	4.586072	3.658374	-2.059165
6	4.545698	-3.937591	1.311662
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6	4.329320	4.118339	0.749971
6	4.201049	3.620457	2.094758
6	4.087039	-3.175612	-2.763975
6	3.940524	-2.074101	-3.678447
6	3.939935	1.433173	3.913348
6	3.805402	0.020547	4.156912
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6	3.523130	-2.652178	3.185978
6	3.374622	-3.583169	2.095229
6	3.272373	3.917906	-1.498822
6	3.144892	4.189818	-0.087367
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6	2.916294	-3.657714	-2.053735
6	2.888552	3.277248	2.606360
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6	2.622924	-1.526406	-3.930611

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6	2.491735	-0.587142	4.127452
6	2.351852	-1.955850	3.675737
6	2.219800	2.583195	-3.321951
6	2.092037	3.548436	-2.249152
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6	1.837484	4.160338	0.527755
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6	1.600558	-3.328492	-2.549138
6	1.453752	-2.274499	-3.530904
6	1.451682	1.656814	3.846346
6	1.318438	0.254470	4.175053
6	1.175072	0.492190	-4.176369
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6	1.038188	-2.468769	3.363700
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6	-8.928774	-1.647678	3.951110
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6	-9.824749	-2.534440	-3.178638
6	-9.957130	-1.264318	-3.866677
6	-9.971270	0.601221	4.288087
6	-10.094812	-0.876688	4.277351
6	-10.248654	1.581507	-3.870850
6	-10.367254	2.851019	-3.118880
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6	-10.992926	2.638538	3.321819
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B3LYP/STO-3G Energy: -9124.721368

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6	11.448019	-1.788991	-3.832174
6	11.331458	-0.407748	-4.133110
6	11.243522	-0.368140	4.244263
6	11.125107	-1.719877	3.823716
6	11.075022	2.358111	-3.402640
6	10.937354	3.400197	-2.392156
6	10.861742	-3.780739	1.838411
6	10.720963	-4.203428	0.446650
6	10.651181	4.225457	0.348233
6	10.510680	3.886833	1.769114
6	10.440900	-3.572941	-2.343675
6	10.315432	-2.539846	-3.395545
6	10.237569	1.924382	3.851990
6	10.113017	0.499827	4.243283
6	10.025092	0.212173	-4.119893
6	9.899990	1.616407	-3.779258
6	9.818283	-2.251179	3.510297
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6	9.628497	3.695219	-1.866697
6	9.486913	4.136616	-0.490154
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6	8.650405	-1.501384	3.897963
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6	8.445044	3.227151	-2.565991
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6	8.162418	4.165918	0.108375
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6	5.954053	3.092783	-2.764021
6	5.880198	-3.532423	2.252740
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6	4.915735	1.175611	-3.972556
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6	2.214356	-2.849723	3.096150
6	2.148714	3.333851	-2.494200
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6	1.935152	-4.154479	0.572409
6	1.795030	-4.095454	-0.867698
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6	0.902450	-3.262191	2.653470
6	0.762322	-3.956686	1.396188
6	0.696474	4.133321	-0.624921
6	0.555677	4.112900	0.809761
6	0.480977	-3.917236	-1.445772
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6	0.137518	1.422521	3.968128
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6	-12.355819	-1.559738	-3.997726
6	-12.509770	0.791513	4.032876
6	-12.635634	-0.576970	4.057596
1	13.628860	-1.080105	-4.107165
1	13.409357	1.382633	-4.090160
1	13.347522	-1.146561	4.297425
1	13.135533	-3.288884	3.082647
1	13.207112	3.175816	-2.925506
1	12.945912	4.439452	-0.837149
1	12.953612	-4.319986	1.203857
1	12.737595	-4.391689	-1.239148
1	12.737223	4.339790	1.313009

1	12.487428	3.159234	3.448641
1	12.589369	-3.087789	-2.924336
1	12.319624	1.186199	4.248935
1	-12.319602	1.148329	-4.259364
1	-12.589387	-3.061601	2.951661
1	-12.487433	3.128409	-3.476599
1	-12.737233	4.327877	-1.351534
1	-12.737617	-4.380393	1.278116
1	-12.953624	-4.330473	-1.165422
1	-12.945921	4.446656	0.797637
1	-13.207113	3.201694	2.897177
1	-13.135523	-3.316209	-3.053383
1	-13.347490	-1.184776	-4.287194
1	-13.409341	1.418983	4.077836
1	-13.628852	-1.043503	4.116717

Nanotube (7,5) ul0v03
B3LYP/STO-3G Energy: -9275.311666

6	12.709530	-3.847864	1.596378
6	12.578182	-4.180196	0.269271
6	12.497204	4.191828	0.451176
6	12.374615	3.836049	1.774166
6	12.270983	-3.358751	-2.615598
6	12.131066	-2.399047	-3.598146
6	12.081974	1.725897	3.910336
6	11.949060	0.404321	4.295718
6	11.834704	0.506938	-4.355736
6	11.705143	1.843227	-4.013877
6	11.672793	-2.445192	3.411687
6	11.550448	-3.391039	2.363188
6	11.445800	3.866661	-1.814194
6	11.333031	4.171549	-0.432445
6	11.280256	-4.128152	-0.399432
6	11.136492	-3.765964	-1.803120
6	11.081578	3.467461	2.342049
6	10.945718	2.467749	3.397342
6	10.842451	-1.791528	-3.873934
6	10.700956	-0.390315	-4.281452
6	10.669264	-0.269557	4.230343
6	10.541525	-1.693556	3.854184
6	10.431280	2.391328	-3.606597
6	10.310958	3.436272	-2.563598
6	10.240687	-3.687204	1.824898
6	10.108590	-4.087525	0.437515
6	10.028222	4.163577	0.190076
6	9.905913	3.833844	1.597183
6	9.825148	-3.454862	-2.314014
6	9.679591	-2.476735	-3.377877
6	9.638755	1.937115	3.691859
6	9.501948	0.561250	4.136660
6	9.396691	0.214290	-4.243928
6	9.261277	1.625357	-3.931550
6	9.221968	-2.198519	3.526772
6	9.075119	-3.242289	2.544767
6	8.994651	3.709545	-2.018598
6	8.856802	4.129445	-0.648190
6	8.787862	-4.110779	-0.158890
6	8.645102	-3.830177	-1.556078
6	8.588107	3.559356	2.136700
6	8.453648	2.630992	3.218562
6	8.354571	-1.970510	-3.693631
6	8.212483	-0.627376	-4.167394
6	8.175365	-0.040671	4.165197
6	8.037074	-1.443055	3.905181
6	7.935869	2.159290	-3.643011
6	7.804003	3.243925	-2.715457
6	7.752325	-3.583184	2.042995

6	7.611744	-4.061888	0.694644
6	7.537720	4.179870	-0.034949
6	7.407140	3.933697	1.376605
6	7.322909	-3.583806	-2.103216
6	7.178572	-2.674283	-3.212540
6	7.135792	2.144707	3.582305
6	6.999094	0.803513	4.100742
6	6.894953	-0.025636	-4.227616
6	6.758341	1.396982	-4.002575
6	6.721067	-1.997486	3.657487
6	6.579601	-3.113621	2.746411
6	6.492154	3.601424	-2.216233
6	6.359989	4.118977	-0.869421
6	6.296740	-4.138028	0.097563
6	6.153833	-3.933324	-1.329064
6	6.097108	3.704808	1.942466
6	5.963569	2.825020	3.085519
6	5.866705	-2.195190	-3.573758
6	5.725479	-0.863290	-4.125034
6	5.688382	0.204131	4.178985
6	5.549496	-1.223380	3.992864
6	5.449739	1.952874	-3.758480
6	5.316026	3.095901	-2.883338
6	5.267555	-3.477418	2.264296
6	5.125760	-4.033210	0.939182
6	5.051844	4.195543	-0.261442
6	4.920248	4.025701	1.165520
6	4.837942	-3.704892	-1.884475
6	4.694086	-2.858792	-3.042018
6	4.649987	2.349586	3.463992
6	4.512380	1.042487	4.052444
6	4.409466	-0.263540	-4.202707
6	4.270906	1.161594	-4.058620
6	4.232669	-1.785697	3.767256
6	4.091048	-2.948029	2.930209
6	4.001203	3.470759	-2.398460
6	3.868558	4.064739	-1.094129
6	3.806229	-4.128363	0.343476
6	3.662290	-4.004262	-1.084327
6	3.604545	3.815173	1.740542
6	3.470178	3.003296	2.923570
6	3.374726	-2.394265	-3.426721
6	3.232664	-1.101546	-4.050996
6	3.195683	0.445482	4.163836
6	3.056227	-0.987764	4.061855
6	2.955488	1.733054	-3.847528
6	2.820553	2.925550	-3.042570
6	2.774269	-3.342460	2.472177
6	2.632049	-3.978364	1.181294
6	2.556497	4.180837	-0.491904
6	2.425214	4.096578	0.946794
6	2.346031	-3.813639	-1.654721
6	2.202972	-3.031676	-2.864414
6	2.158440	2.553778	3.334063
6	2.022015	1.274997	3.998627
6	1.920398	-0.509500	-4.170471
6	1.781729	0.930044	-4.107517
6	1.744176	-1.562818	3.876563
6	1.602919	-2.778615	3.105089
6	1.511700	3.329330	-2.585143
6	1.379098	4.001716	-1.311508
6	1.318475	-4.106849	0.593899
6	1.175025	-4.063898	-0.843336
6	1.116134	3.916550	1.530597
6	0.982540	3.170370	2.759524
6	0.889073	-2.588478	-3.271581
6	0.747152	-1.332921	-3.967372
6	0.709827	0.685194	4.139435
6	0.570192	-0.749390	4.118417
6	0.468822	1.508932	-3.923751

6	0.332477	2.741257	-3.190291
6	0.286910	-3.192709	2.666727
6	0.143543	-3.899444	1.420043
6	0.066078	4.143395	-0.715660
6	-0.066078	4.142975	0.718094
6	-0.143543	-3.898608	-1.422333
6	-0.286910	-3.191141	-2.668601
6	-0.332477	2.739381	3.191900
6	-0.468822	1.506625	3.924636
6	-0.570193	-0.746969	-4.118855
6	-0.709827	0.687627	-4.139032
6	-0.747152	-1.335253	3.966589
6	-0.889072	-2.590401	3.270061
6	-0.982539	3.171992	-2.757662
6	-1.116134	3.917450	-1.528297
6	-1.175025	-4.064393	0.840949
6	-1.318474	-4.106500	-0.596311
6	-1.379099	4.000944	1.313858
6	-1.511700	3.327810	2.587097
6	-1.602919	-2.776788	-3.106719
6	-1.744176	-1.560538	-3.877479
6	-1.781730	0.927630	4.108062
6	-1.920398	-0.511951	4.170172
6	-2.022014	1.277348	-3.997878
6	-2.158440	2.555738	-3.332563
6	-2.202972	-3.033361	2.862635
6	-2.346030	-3.814613	1.652482
6	-2.425213	4.097135	-0.944388
6	-2.556497	4.180547	0.494360
6	-2.632049	-3.977669	-1.183629
6	-2.774270	-3.341005	-2.474138
6	-2.820554	2.923760	3.044287
6	-2.955489	1.730791	3.848544
6	-3.056227	-0.985376	-4.062433
6	-3.195682	0.447930	-4.163573
6	-3.232663	-1.103928	4.050349
6	-3.374725	-2.396280	3.425316
6	-3.470177	3.005016	-2.921807
6	-3.604544	3.816198	-1.738302
6	-3.662290	-4.004901	1.081976
6	-3.806229	-4.128160	-0.345899
6	-3.868559	4.064095	1.096515
6	-4.001204	3.469347	2.400496
6	-4.091049	-2.946304	-2.931937
6	-4.232670	-1.783481	-3.768301
6	-4.270907	1.159208	4.059300
6	-4.409466	-0.266012	4.202551
6	-4.512379	1.044870	-4.051832
6	-4.649985	2.351624	-3.462614
6	-4.694085	-2.860582	3.040341
6	-4.837940	-3.706002	1.882302
6	-4.920247	4.026389	-1.163158
6	-5.051844	4.195388	0.263904
6	-5.125760	-4.032657	-0.941548
6	-5.267556	-3.476083	-2.266335
6	-5.316028	3.094202	2.885152
6	-5.449741	1.950662	3.759622
6	-5.549497	-1.221030	-3.993578
6	-5.688382	0.206589	-4.178863
6	-5.725479	-0.865716	4.124527
6	-5.866704	-2.197293	3.572472
6	-5.963567	2.826838	-3.083863
6	-6.097107	3.705954	-1.940294
6	-6.153831	-3.934108	1.326757
6	-6.296739	-4.137970	-0.099991
6	-6.359990	4.118464	0.871837
6	-6.492156	3.600116	2.218343
6	-6.579603	-3.112002	-2.748233
6	-6.721069	-1.995332	-3.658653
6	-6.758343	1.394626	4.003391

6	-6.894954	-0.028124	4.227600
6	-6.999093	0.805927	-4.100270
6	-7.135790	2.146818	-3.581051
6	-7.178570	-2.676177	3.210974
6	-7.322907	-3.585048	2.101116
6	-7.407139	3.934512	-1.374300
6	-7.537720	4.179851	0.037400
6	-7.611744	-4.061478	-0.697025
6	-7.752327	-3.581978	-2.045093
6	-7.804006	3.242322	2.717355
6	-7.935872	2.157142	3.644272
6	-8.037075	-1.440754	-3.906022
6	-8.175365	-0.038218	-4.165219
6	-8.212482	-0.629830	4.167027
6	-8.354569	-1.972687	3.692480
6	-8.453646	2.632892	-3.217025
6	-8.588105	3.560621	-2.134618
6	-8.645100	-3.831098	1.553835
6	-8.787861	-4.110874	0.156481
6	-8.856804	4.129062	0.650608
6	-8.994653	3.708350	2.020767
6	-9.075121	-3.240785	-2.546662
6	-9.221970	-2.196438	-3.528053
6	-9.261279	1.623038	3.932497
6	-9.396692	0.211789	4.244052
6	-9.501947	0.563688	-4.136332
6	-9.638753	1.939294	-3.690730
6	-9.679589	-2.478731	3.376431
6	-9.825145	-3.456233	2.311994
6	-9.905912	3.834792	-1.594941
6	-10.028222	4.163690	-0.187639
6	-10.108591	-4.087266	-0.439909
6	-10.240689	-3.686122	-1.827053
6	-10.310961	3.434753	2.565603
6	-10.431283	2.389196	3.607988
6	-10.541527	-1.691280	-3.855167
6	-10.669264	-0.267063	-4.230498
6	-10.700956	-0.392840	4.281222
6	-10.842449	-1.793816	3.872890
6	-10.945715	2.469758	-3.395906
6	-11.081575	3.468850	-2.340026
6	-11.136489	-3.767037	1.800919
6	-11.280255	-4.128391	0.397017
6	-11.333033	4.171289	0.434884
6	-11.445804	3.865579	1.816452
6	-11.550450	-3.389636	-2.365165
6	-11.672796	-2.443171	-3.413106
6	-11.705146	1.840855	4.014943
6	-11.834706	0.504367	4.356024
6	-11.949058	0.406856	-4.295487
6	-12.081971	1.728207	-3.909337
6	-12.131063	-2.401180	3.596752
6	-12.270979	-3.360307	2.613642
6	-12.374614	3.837102	-1.771927
6	-12.497205	4.192094	-0.448726
6	-12.578182	-4.180035	-0.271714
6	-12.709532	-3.846912	-1.598624
1	13.703986	-3.792373	2.060547
1	13.474545	-4.396053	-0.326451
1	13.489407	4.365943	0.012201
1	13.275954	3.731088	2.391831
1	13.274638	-3.718189	-2.354907
1	13.025990	-2.011143	-4.101698
1	13.083564	2.171893	3.861123
1	12.848904	-0.173294	4.544068
1	12.835622	0.097506	-4.543283
1	12.607378	2.463882	-3.937947
1	12.682302	-2.130618	3.705626
1	12.452863	3.737706	-2.231023
1	-12.452865	3.736376	2.233202

1	-12.682304	-2.128421	-3.706857
1	-12.607383	2.461552	3.939369
1	-12.835624	0.094823	4.543327
1	-12.848903	-0.170612	-4.544177
1	-13.083560	2.174178	-3.859869
1	-13.025986	-2.013578	4.100537
1	-13.274633	-3.719600	2.352746
1	-13.275951	3.732508	-2.389657
1	-13.489408	4.365947	-0.009649
1	-13.474545	-4.396244	0.323881
1	-13.703989	-3.791142	-2.062757

Nanotube (7,5) u10v04
B3LYP/STO-3G Energy: -9350.606631

6	12.829523	3.238522	-2.563992
6	12.707643	3.901510	-1.366429
6	12.571588	-4.236557	0.603382
6	12.443428	-4.231861	-0.765916
6	12.411107	3.851892	1.633939
6	12.270589	3.177707	2.830210
6	12.152236	-2.737867	-3.370694
6	12.025873	-1.558244	-4.081029
6	11.960448	0.564836	4.307753
6	11.820677	-0.813155	4.319729
6	11.773590	1.424941	-3.954666
6	11.663233	2.608553	-3.183444
6	11.535849	-3.331168	2.713106
6	11.412827	-3.979747	1.456984
6	11.413045	4.032709	-0.701762
6	11.274616	4.044684	0.747855
6	11.149409	-4.010588	-1.404282
6	11.013905	-3.314398	-2.679759
6	10.979562	2.670347	3.257202
6	10.831638	1.421872	4.010375
6	10.750758	-0.879771	-4.185199
6	10.634605	0.593514	-4.185723
6	10.540810	-1.437830	4.071252
6	10.407838	-2.713815	3.331800
6	10.358259	3.043237	-2.734378
6	10.236316	3.787468	-1.496128
6	10.104203	-4.122027	0.858555
6	9.975561	-4.164190	-0.585342
6	9.963986	3.885423	1.326519
6	9.818080	3.214450	2.606414
6	9.708619	-2.866940	-3.095616
6	9.578359	-1.650021	-3.877730
6	9.523339	0.837713	4.134463
6	9.377408	-0.605337	4.194483
6	9.320366	1.175919	-3.994142
6	9.185873	2.437821	-3.311988
6	9.086805	-3.108122	2.880878
6	8.938086	-3.864873	1.664694
6	8.919255	3.973512	-0.920968
6	8.782281	4.062309	0.502045
6	8.656610	-4.027298	-1.171950
6	8.521826	-3.406758	-2.455469
6	8.491921	2.816121	3.046379
6	8.344132	1.640477	3.849277
6	8.255919	-1.065172	-4.054381
6	8.128496	0.357983	-4.161789
6	8.047391	-1.185311	4.057636
6	7.903347	-2.470161	3.439671
6	7.868377	2.906241	-2.909573
6	7.738181	3.715787	-1.728988
6	7.615272	-4.060665	1.090216
6	7.477678	-4.184113	-0.336249
6	7.461551	3.974262	1.098930

6	7.317449	3.381337	2.404649
6	7.205018	-3.019359	-2.926273
6	7.074171	-1.855480	-3.770622
6	7.023077	1.083995	4.066504
6	6.876371	-0.347022	4.214312
6	6.817513	0.967724	-4.059564
6	6.688460	2.280807	-3.464973
6	6.586156	-2.933930	3.054152
6	6.442568	-3.778374	1.886275
6	6.426766	3.952784	-1.166577
6	6.290076	4.122195	0.264950
6	6.165472	-4.097884	-0.936670
6	6.030781	-3.540242	-2.266505
6	6.004305	3.020900	2.881722
6	5.857836	1.876450	3.757076
6	5.766896	-1.285955	-3.995259
6	5.638750	0.142536	-4.181347
6	5.562944	-0.937230	4.126862
6	5.417102	-2.265642	3.574831
6	5.381641	2.766740	-3.088046
6	5.250593	3.644971	-1.949207
6	5.130472	-3.998795	1.323828
6	4.991163	-4.199679	-0.098629
6	4.975942	4.054015	0.865116
6	4.832942	3.534352	2.201787
6	4.718314	-3.167616	-2.749074
6	4.586077	-2.054296	-3.653179
6	4.539020	1.326641	3.991271
6	4.391020	-0.086729	4.218640
6	4.327451	0.754295	-4.103080
6	4.198301	2.093611	-3.591837
6	4.097693	-2.742503	3.207895
6	3.953370	-3.649738	2.100020
6	3.935277	3.899647	-1.393044
6	3.797900	4.146452	0.019110
6	3.673610	-4.132723	-0.702843
6	3.537252	-3.650515	-2.053636
6	3.512838	3.193290	2.697238
6	3.366173	2.106022	3.632925
6	3.272912	-1.495231	-3.908722
6	3.143864	-0.083434	-4.178238
6	3.070937	-0.683569	4.166488
6	2.924082	-2.041033	3.695713
6	2.886759	2.602810	-3.245663
6	2.755421	3.548885	-2.160805
6	2.636753	-3.906094	1.552961
6	2.496802	-4.191619	0.141936
6	2.483111	4.117827	0.623956
6	2.341284	3.673491	1.993804
6	2.225614	-3.310430	-2.560181
6	2.093967	-2.244990	-3.530582
6	2.050648	1.574266	3.905881
6	1.903075	0.168252	4.216591
6	1.836745	0.530648	-4.142982
6	1.708108	1.904890	-3.709667
6	1.610067	-2.539674	3.363653
6	1.465450	-3.514956	2.305304
6	1.445868	3.834139	-1.621658
6	1.309365	4.161078	-0.220534
6	1.185157	-4.156816	-0.462845
6	1.048733	-3.749140	-1.841634
6	1.027023	3.359272	2.505659
6	0.881251	2.325798	3.501864
6	0.785236	-1.700820	-3.813764
6	0.655929	-0.307979	-4.163462
6	0.586432	-0.428896	4.194160
6	0.438633	-1.807765	3.803267
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6	0.265707	3.431873	-2.363594
6	0.148592	-3.794454	1.771559

6	0.006930	-4.158405	0.385616
6	-0.006930	4.158387	0.385801
6	-0.148592	3.794375	1.771728
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6	-0.655929	0.308162	-4.163448
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6	-1.465450	3.514853	2.305460
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6	-7.074170	1.855649	-3.770539

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6	-9.086805	3.107994	2.881012
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6	-9.320367	-1.175740	-3.994187
6	-9.377409	0.605150	4.194505
6	-9.523340	-0.837898	4.134423
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1	12.718415	-1.439478	4.402216
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B3LYP/STO-3G Energy: -9425.901494

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6	11.898342	-0.415004	4.143076
6	11.777272	-1.755166	3.700042
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6	11.526600	3.420362	-2.469014
6	11.503152	-3.765644	1.666700
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6	10.900259	-2.449976	-3.553621
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6	10.502054	1.723849	-3.952396
6	10.467064	-2.282205	3.384268
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6	10.222635	3.720184	-1.920181
6	10.103843	4.132641	-0.535103
6	10.040036	-4.135508	-0.322607
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6	6.552324	3.149314	-2.806919
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6	6.372624	-4.068418	0.785534
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6	-6.805807	-1.335189	-3.916662
6	-6.944878	0.084967	-4.154473
6	-6.952334	-0.766483	4.180812
6	-7.092941	-2.112323	3.672309
6	-7.212471	2.738260	-3.150392

6	-7.343419	3.645370	-2.035428
6	-7.388114	-3.908191	1.478326
6	-7.539074	-4.146859	0.065427
6	-7.604612	4.104358	0.768261
6	-7.732143	3.618327	2.115681
6	-7.837137	-3.173348	-2.600061
6	-7.979337	-2.089607	-3.533167
6	-7.995845	1.477376	3.981163
6	-8.128968	0.076451	4.250842
6	-8.259453	0.692500	-4.090525
6	-8.392695	2.039867	-3.621723
6	-8.412869	-2.603580	3.327659
6	-8.560751	-3.534831	2.250761
6	-8.658957	3.890965	-1.474283
6	-8.788362	4.160015	-0.073640
6	-8.863544	-4.087300	-0.526547
6	-9.011185	-3.637005	-1.878382
6	-9.049804	3.273056	2.627710
6	-9.186324	2.229127	3.610547
6	-9.301445	-1.542086	-3.795031
6	-9.446336	-0.148483	-4.131349
6	-9.454782	-0.528043	4.242368
6	-9.593900	-1.908650	3.815843
6	-9.716380	2.551715	-3.294408
6	-9.847290	3.526250	-2.225440
6	-9.887952	-3.815391	1.730887
6	-10.040036	-4.135513	0.322439
6	-10.103844	4.132612	0.535265
6	-10.222637	3.720099	1.920326
6	-10.332979	-3.317561	-2.378810
6	-10.467063	-2.282067	-3.384367
6	-10.502055	1.723690	3.952470
6	-10.623368	0.300753	4.342154
6	-10.764444	0.455397	-4.160379
6	-10.887382	1.878376	-3.782781
6	-10.900259	-2.450119	3.553528
6	-11.047522	-3.464155	2.506395
6	-11.152087	3.843362	-1.701713
6	-11.282633	4.186834	-0.289813
6	-11.354209	-4.148729	-0.270262
6	-11.503151	-3.765570	-1.666856
6	-11.526602	3.420256	2.469149
6	-11.637735	2.471431	3.517960
6	-11.777270	-1.755014	-3.700117
6	-11.898342	-0.414832	-4.143089
6	-11.898468	-0.375469	4.430393
6	-12.031338	-1.705357	4.067423
6	-12.165104	2.500173	-3.502181
6	-12.292316	3.457146	-2.512467
6	-12.339285	-3.853571	1.970866
6	-12.485253	-4.198232	0.642393
6	-12.573541	4.228023	0.390841
6	-12.692482	3.879988	1.715955
6	-12.803055	-3.476361	-2.268380
6	-12.936363	-2.529805	-3.255665
1	13.931645	-2.250060	3.627744
1	13.698715	-3.957745	1.854593
1	13.683074	3.816547	-2.187024
1	13.476189	4.446729	0.194444
1	13.490544	-4.380665	-0.242075
1	13.231147	-3.766670	-2.605046
1	13.291752	3.823904	2.246381
1	13.067220	2.124536	4.002541
1	13.032733	-2.152997	-4.032951
1	12.798597	0.203044	-4.676060
1	12.907414	0.006290	4.240074
1	12.644364	2.155481	-3.820675
1	-12.644368	2.155330	3.820771
1	-12.907422	0.006476	-4.240032
1	-12.798595	0.202849	4.676096

1	-13.032734	-2.153167	4.032880
1	-13.067215	2.124694	-4.002464
1	-13.291753	3.823989	-2.246233
1	-13.231151	-3.766760	2.604889
1	-13.490539	-4.380668	0.241899
1	-13.476192	4.446709	-0.194276
1	-13.683076	3.816440	2.187165
1	-13.698714	-3.957663	-1.854756
1	-13.931646	-2.249899	-3.627834

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B3LYP/STO-3G Energy: -9501.198307

6	-13.005531	-1.557198	-3.859615
6	-12.883096	-2.731565	-3.148007
6	-12.783097	3.346406	2.598309
6	-12.653203	4.027484	1.405313
6	-12.589279	-4.186201	-0.524654
6	-12.452423	-4.198303	0.854353
6	-12.350552	4.034992	-1.594992
6	-12.218368	3.361698	-2.802276
6	-12.155249	-2.663812	3.434646
6	-12.022033	-1.466967	4.131256
6	-11.954998	0.709710	-4.174040
6	-11.843001	-0.709219	-4.089717
6	-11.747218	1.519213	3.989540
6	-11.627022	2.713863	3.217080
6	-11.593304	-3.176801	-2.642514
6	-11.456018	-3.914351	-1.382226
6	-11.362075	4.164755	0.751821
6	-11.221069	4.196350	-0.710325
6	-11.170052	-3.970708	1.478632
6	-11.027793	-3.255386	2.760457
6	-10.947472	2.830313	-3.224287
6	-10.825862	1.543805	-3.958115
6	-10.752114	-0.799190	4.229533
6	-10.624252	0.683391	4.219926
6	-10.541145	-1.303513	-3.907178
6	-10.418627	-2.563728	-3.199872
6	-10.321935	3.134576	2.770217
6	-10.191697	3.888556	1.538528
6	-10.148629	-4.052609	-0.796853
6	-10.006310	-4.105950	0.645963
6	-9.914572	4.009769	-1.285659
6	-9.777691	3.342280	-2.565804
6	-9.722704	-2.799036	3.154556
6	-9.583190	-1.576527	3.920124
6	-9.506207	0.945764	-4.069928
6	-9.367658	-0.486258	-4.103308
6	-9.300292	1.251597	4.024214
6	-9.153141	2.512561	3.346467
6	-9.098188	-3.008150	-2.790164
6	-8.962063	-3.794244	-1.598936
6	-8.867957	4.067086	0.966854
6	-8.727981	4.167423	-0.457467
6	-8.679291	-3.978104	1.229751
6	-8.536921	-3.354713	2.515151
6	-8.450488	2.930612	-3.008284
6	-8.317780	1.743173	-3.812529
6	-8.254339	-1.003565	4.099593
6	-8.116188	0.427538	4.202986
6	-8.050630	-1.089394	-3.988791
6	-7.920222	-2.386396	-3.362241
6	-7.833071	2.975492	2.955398
6	-7.695077	3.797437	1.771862
6	-7.647462	-4.015159	-1.036972
6	-7.507232	-4.149003	0.400615
6	-7.415073	4.072263	-1.052896

6	-7.278816	3.476385	-2.370784
6	-7.225774	-2.977098	2.983089
6	-7.086386	-1.799881	3.825253
6	-7.010682	1.167850	-4.019162
6	-6.877673	-0.271608	-4.153148
6	-6.806707	1.023213	4.100386
6	-6.665328	2.339226	3.504326
6	-6.613038	-2.863837	-2.985535
6	-6.477192	-3.721091	-1.826031
6	-6.385148	4.018593	1.211279
6	-6.245390	4.193607	-0.218722
6	-6.197964	-4.061552	0.995288
6	-6.056447	-3.501293	2.321044
6	-5.967941	3.091923	-2.838453
6	-5.832984	1.946155	-3.706134
6	-5.773369	-1.238252	4.039821
6	-5.632454	0.186785	4.220279
6	-5.566514	-0.876270	-4.060019
6	-5.433645	-2.202793	-3.508811
6	-5.349812	2.812940	3.129212
6	-5.209058	3.694545	1.995528
6	-5.160315	-3.957047	-1.267938
6	-5.020129	-4.169709	0.152376
6	-4.926902	4.116015	-0.817836
6	-4.788358	3.596950	-2.158710
6	-4.737210	-3.139572	2.803078
6	-4.596131	-2.020455	3.706822
6	-4.518183	1.382724	-3.942540
6	-4.385564	-0.041047	-4.165871
6	-4.315071	0.787228	4.150553
6	-4.174508	2.134611	3.637982
6	-4.120779	-2.699950	-3.155438
6	-3.984993	-3.621292	-2.044271
6	-3.894479	3.945658	1.446379
6	-3.754508	4.198114	0.024549
6	-3.707646	-4.119357	0.754025
6	-3.566809	-3.633492	2.114694
6	-3.478498	3.243913	-2.652129
6	-3.343707	2.145010	-3.589831
6	-3.285542	-1.473683	3.960503
6	-3.145053	-0.054520	4.226730
6	-3.079102	-0.649542	-4.112194
6	-2.946502	-2.012582	-3.638410
6	-2.864544	2.629794	3.293043
6	-2.723862	3.578655	2.207937
6	-2.675530	-3.887005	-1.499998
6	-2.536012	-4.177479	-0.089557
6	-2.442833	4.149868	-0.577132
6	-2.303681	3.704129	-1.944855
6	-2.254159	-3.295901	2.613088
6	-2.112370	-2.230174	3.578062
6	-2.032821	1.595204	-3.852570
6	-1.899440	0.190649	-4.158892
6	-1.830444	0.547071	4.185743
6	-1.688975	1.917839	3.754639
6	-1.633396	-2.523660	-3.306830
6	-1.497052	-3.502241	-2.253888
6	-1.406996	3.852365	1.670667
6	-1.265671	4.181581	0.270909
6	-1.219054	-4.155013	0.513760
6	-1.077673	-3.748598	1.893854
6	-0.988360	3.377803	-2.456201
6	-0.852714	2.338561	-3.453860
6	-0.795924	-1.699131	3.863227
6	-0.655095	-0.301118	4.213716
6	-0.587708	-0.419866	-4.143893
6	-0.454992	-1.808947	-3.753191
6	-0.374600	2.434214	3.443369
6	-0.233820	3.446230	2.414322
6	-0.185088	-3.803309	-1.727693

6	-0.046333	-4.173308	-0.332110
6	0.046336	4.173265	-0.332637
6	0.185090	3.803088	-1.728172
6	0.233821	-3.445921	2.414756
6	0.374600	-2.433775	3.443675
6	0.454989	1.808470	-3.753419
6	0.587704	0.419340	-4.143947
6	0.655093	0.301653	4.213680
6	0.795922	1.699622	3.863015
6	0.852712	-2.339001	-3.453568
6	0.988359	-3.378115	-2.455777
6	1.077675	3.748838	1.893381
6	1.219057	4.155076	0.513236
6	1.265674	-4.181544	0.271436
6	1.406999	-3.852149	1.671153
6	1.497052	3.501950	-2.254329
6	1.633394	2.523237	-3.307149
6	1.688974	-1.917361	3.754882
6	1.830442	-0.546539	4.185816
6	1.899435	-0.191178	-4.158873
6	2.032817	-1.595694	-3.852375
6	2.112368	2.230629	3.577785
6	2.254159	3.296232	2.612675
6	2.303681	-3.704374	-1.944390
6	2.442836	-4.149936	-0.576610
6	2.536015	4.177461	-0.090084
6	2.675532	3.886808	-1.500488
6	2.723864	-3.578369	2.208388
6	2.864545	-2.629373	3.293375
6	2.946499	2.012118	-3.638667
6	3.079098	0.649019	-4.112284
6	3.145051	0.055058	4.226731
6	3.285540	1.474187	3.960325
6	3.343703	-2.145467	-3.589569
6	3.478497	-3.244249	-2.651725
6	3.566810	3.633757	2.114237
6	3.707648	4.119445	0.753505
6	3.754511	-4.198102	0.025077
6	3.894482	-3.945464	1.446875
6	3.984995	3.621023	-2.044728
6	4.120778	2.699544	-3.155782
6	4.174508	-2.134146	3.638255
6	4.315069	-0.786700	4.150661
6	4.385559	0.040517	-4.165889
6	4.518178	-1.383226	-3.942379
6	4.596129	2.020927	3.706577
6	4.737210	3.139926	2.802687
6	4.788358	-3.597220	-2.158261
6	4.926904	-4.116109	-0.817319
6	5.020133	4.169716	0.151850
6	5.160318	3.956872	-1.268437
6	5.209062	-3.694280	1.995992
6	5.349814	-2.812535	3.129568
6	5.433644	2.202343	-3.509095
6	5.566510	0.875752	-4.060143
6	5.632452	-0.186247	4.220316
6	5.773366	1.238767	4.039680
6	5.832980	-1.946628	-3.705905
6	5.967939	-3.092282	-2.838073
6	6.056448	3.501583	2.320606
6	6.197967	4.061665	0.994776
6	6.245393	-4.193619	-0.218196
6	6.385152	-4.018421	1.211782
6	6.477194	3.720843	-1.826500
6	6.613039	2.863447	-2.985900
6	6.665329	-2.338774	3.504625
6	6.806705	-1.022689	4.100528
6	6.877668	0.271078	-4.153203
6	7.010677	-1.168363	-4.019037
6	7.086383	1.800370	3.825043

6	7.225773	2.977476	2.982723
6	7.278815	-3.476682	-2.370356
6	7.415075	-4.072382	-1.052387
6	7.507235	4.149035	0.400092
6	7.647465	4.015006	-1.037477
6	7.695082	-3.797191	1.772337
6	7.833074	-2.975103	2.955773
6	7.920221	2.385959	-3.362550
6	8.050627	1.088883	-3.988948
6	8.116185	-0.427001	4.203060
6	8.254335	1.004090	4.099490
6	8.317775	-1.743661	-3.812335
6	8.450485	-2.930994	-3.007933
6	8.536921	3.355027	2.514736
6	8.679294	3.978243	1.229252
6	8.727984	-4.167459	-0.456947
6	8.867962	-4.066936	0.967360
6	8.962066	3.794016	-1.599413
6	9.098189	3.007778	-2.790547
6	9.153143	-2.512123	3.346788
6	9.300290	-1.251079	4.024389
6	9.367654	0.485731	-4.103396
6	9.506202	-0.946286	-4.069841
6	9.583186	1.577030	3.919952
6	9.722702	2.799436	3.154220
6	9.777689	-3.342602	-2.565400
6	9.914574	-4.009914	-1.285163
6	10.006314	4.106006	0.645448
6	10.148633	4.052476	-0.797362
6	10.191702	-3.888329	1.539010
6	10.321939	-3.134201	2.770608
6	10.418627	2.563306	-3.200204
6	10.541142	1.303009	-3.907365
6	10.624249	-0.682848	4.220038
6	10.752109	0.799735	4.229467
6	10.825856	-1.544314	-3.957956
6	10.947468	-2.830726	-3.223957
6	11.027792	3.255731	2.760062
6	11.170055	3.970873	1.478137
6	11.221072	-4.196412	-0.709806
6	11.362081	-4.164622	0.752336
6	11.456023	3.914139	-1.382717
6	11.593306	3.176439	-2.642918
6	11.627025	-2.713431	3.217421
6	11.747217	-1.518692	3.989748
6	11.842997	0.708691	-4.089839
6	11.954993	-0.710248	-4.173992
6	12.022028	1.467502	4.131113
6	12.155246	2.664254	3.434341
6	12.218366	-3.362052	-2.801876
6	12.350553	-4.035176	-1.594498
6	12.452428	4.198373	0.853828
6	12.589284	4.186088	-0.525178
6	12.653210	-4.027258	1.405805
6	12.783103	-3.346036	2.598720
6	12.883097	2.731143	-3.148363
6	13.005529	1.556695	-3.859837
1	-13.998950	-1.180145	-4.139640
1	-13.786556	-3.288377	-2.867766
1	-13.779444	3.156872	3.021185
1	-13.553891	4.379983	0.886308
1	-13.594518	-4.242039	-0.961436
1	-13.352381	-4.261671	1.479617
1	-13.353768	4.313608	-1.247934
1	-13.121648	3.122561	-3.378413
1	-13.160112	-3.074011	3.271360
1	-12.926662	-0.964457	4.497520
1	-12.963303	1.143070	-4.158946
1	-12.758387	1.139999	4.185797
1	12.758385	-1.139452	4.185960

1	12.963297	-1.143607	-4.158847
1	12.926655	0.965045	4.497453
1	13.160109	3.074434	3.271009
1	13.121644	-3.122995	-3.378051
1	13.353770	-4.313745	-1.247405
1	13.352386	4.261812	1.479083
1	13.594525	4.241858	-0.961966
1	13.553899	-4.379808	0.886838
1	13.779449	-3.156440	3.021568
1	13.786558	3.287987	-2.868187
1	13.998947	1.179609	-4.139822

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B3LYP/STO-3G Energy: -9576.496310

6	13.138865	-0.539799	4.066417
6	13.010197	-1.856333	3.679226
6	12.869329	2.540911	-3.441121
6	12.749915	3.503683	-2.460298
6	12.695824	-3.929089	1.513694
6	12.548204	-4.293176	0.185027
6	12.471681	4.279109	0.440690
6	12.348283	3.940174	1.781311
6	12.230577	-3.476038	-2.701587
6	12.092082	-2.499898	-3.682649
6	12.092591	1.734561	3.794185
6	11.978639	0.342475	4.078456
6	11.820228	0.422237	-4.311358
6	11.707386	1.774544	-3.868975
6	11.716070	-2.412031	3.311842
6	11.568907	-3.445441	2.282204
6	11.463987	3.806891	-1.853299
6	11.334907	4.211935	-0.447335
6	11.260519	-4.231442	-0.466993
6	11.108165	-3.870547	-1.888454
6	11.079580	3.540478	2.335780
6	10.962315	2.487968	3.377891
6	10.821253	-1.876835	-3.939935
6	10.694423	-0.441573	-4.311045
6	10.674810	-0.275262	4.063508
6	10.546058	-1.674188	3.702881
6	10.406286	2.299356	-3.534302
6	10.286963	3.343077	-2.534663
6	10.256942	-3.726058	1.761378
6	10.103408	-4.146580	0.381222
6	10.032834	4.184302	0.166440
6	9.905417	3.869342	1.576434
6	9.800098	-3.528747	-2.377179
6	9.654826	-2.544942	-3.431444
6	9.643207	1.942738	3.649551
6	9.503687	0.567986	4.051298
6	9.372823	0.161654	-4.256981
6	9.232382	1.554309	-3.923240
6	9.222403	-2.204927	3.429315
6	9.076853	-3.268544	2.479441
6	8.968212	3.665668	-2.017332
6	8.839940	4.127691	-0.665529
6	8.771833	-4.169704	-0.205934
6	8.619379	-3.897599	-1.606897
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6	8.453421	2.650064	3.203331
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6	8.186445	-0.677514	-4.208416
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6	7.788196	3.202778	-2.717956
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6	7.013859	0.794936	4.061574
6	6.877974	-0.071716	-4.251999
6	6.742730	1.353643	-4.011963
6	6.738551	-2.008981	3.599494
6	6.593571	-3.134143	2.698735
6	6.483083	3.564471	-2.223003
6	6.355243	4.100470	-0.884290
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6	6.097308	3.709497	1.932428
6	5.967953	2.825827	3.066734
6	5.844031	-2.238509	-3.603965
6	5.702494	-0.907352	-4.143468
6	5.701692	0.190080	4.135782
6	5.563810	-1.232935	3.944108
6	5.430968	1.911338	-3.760013
6	5.300568	3.053930	-2.888926
6	5.272358	-3.501735	2.229210
6	5.121137	-4.070660	0.912245
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6	4.912969	4.026039	1.154199
6	4.817127	-3.754615	-1.911914
6	4.668948	-2.905382	-3.071244
6	4.654093	2.345419	3.449094
6	4.521899	1.027704	4.031371
6	4.385594	-0.305251	-4.219096
6	4.250434	1.128312	-4.068444
6	4.247504	-1.800648	3.739163
6	4.102914	-2.975488	2.902595
6	3.990192	3.441518	-2.412369
6	3.862126	4.050372	-1.102195
6	3.803518	-4.173749	0.327769
6	3.651912	-4.053028	-1.110803
6	3.606056	3.815930	1.731615
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6	3.214151	-1.135092	-4.067508
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6	3.077357	-1.009587	4.038227
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6	2.639046	-4.011586	1.166850
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6	1.900531	-0.539335	-4.171086
6	1.763954	0.896322	-4.105385
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6	1.616940	-2.801023	3.093060
6	1.501305	3.302262	-2.586393
6	1.371894	3.979843	-1.317578
6	1.317312	-4.141701	0.587848
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6	-3.990192	3.441567	2.412283
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6	-9.372813	0.161758	4.257014
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6	-10.546057	-1.674278	-3.702867
6	-10.674808	-0.275363	-4.063534
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6	-10.962317	2.487875	-3.377964
6	-11.079586	3.540393	-2.335863
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6	-0.238282	-3.458206	-2.341133
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6	0.587196	-0.404881	4.197679
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6	0.793912	-1.714455	-3.790830
6	0.856400	2.351316	3.499790
6	0.993176	3.388788	2.501104
6	1.072764	-3.762208	-1.819648
6	1.213168	-4.165516	-0.438694
6	1.271019	4.186492	-0.227510
6	1.411675	3.850529	-1.624992
6	1.492071	-3.499521	2.325191
6	1.629786	-2.514554	3.371822
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6	1.831858	0.529393	-4.118868
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6	2.035855	1.607190	3.899532
6	2.109796	-2.247060	-3.503954
6	2.249758	-3.311717	-2.538933
6	2.309067	3.713281	1.988913
6	2.448261	4.156863	0.620780
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6	2.669705	-3.890580	1.573233
6	2.728579	3.572674	-2.161096
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6	2.944470	-2.003247	3.699752
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6	3.146843	-0.074340	-4.155138
6	3.285086	-1.491990	-3.885647
6	3.347791	2.154801	3.635100
6	3.483490	3.252621	2.696144
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6	3.702038	-4.135595	-0.678841
6	3.759440	4.203966	0.018734
6	3.899308	3.945937	-1.402474
6	3.980422	-3.624484	2.116172
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6	4.179241	2.117989	-3.578672
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6	4.387038	-0.031064	4.215924
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6	6.609273	-2.864990	3.051334
6	6.671668	2.322701	-3.443861
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6	6.879444	-0.265263	4.201550
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6	7.086367	-1.825934	-3.741534
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6	7.917650	-2.387544	3.424683
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6	9.156918	2.507186	-3.287089
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6	9.510275	0.947554	4.107993
6	9.576410	-1.605894	-3.810996
6	9.721216	-2.828724	-3.066344
6	9.782543	3.345636	2.604367
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6	10.141625	-4.086683	0.877204
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6	10.415330	-2.572710	3.264840
6	10.540818	-1.305125	3.958187
6	10.618124	0.648900	-4.066485
6	10.745954	-0.795907	-4.051932
6	10.831253	1.543099	3.992892
6	10.953437	2.831856	3.259891
6	11.043015	-3.285143	-2.672507
6	11.170195	-4.029585	-1.393309
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1	13.787907	3.226911	-2.963692
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B3LYP/STO-3G Energy: -9727.091671

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6	-8.254301	-4.047074	-0.655915
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6	-9.442701	4.178634	0.573511
6	-9.589003	3.777514	1.947592
6	-9.702551	-3.235168	-2.525890
6	-9.838248	-2.204169	-3.520717
6	-9.879780	1.718118	3.886630
6	-10.026604	0.314343	4.217228
6	-10.097700	0.551413	-4.166492
6	-10.226325	1.932448	-3.741279
6	-10.326255	-2.387318	3.384976
6	-10.475068	-3.377752	2.334649
6	-10.487944	3.860934	-1.672723
6	-10.612761	4.211327	-0.270865
6	-10.752811	-4.045813	-0.410800
6	-10.876063	-3.664326	-1.804900
6	-10.912454	3.525156	2.492638
6	-11.044191	2.490854	3.553312
6	-11.155469	-1.697317	-3.864127
6	-11.271220	-0.270940	-4.261077
6	-11.334812	-0.279664	4.265037
6	-11.485314	-1.692174	3.873287
6	-11.529335	2.479106	-3.465169
6	-11.662061	3.498872	-2.417787
6	-11.785006	-3.690434	1.826735
6	-11.926243	-4.071743	0.419294
6	-11.916749	4.241531	0.345637
6	-12.035512	3.954669	1.737705
6	-12.178193	-3.370090	-2.353581
6	-12.287969	-2.433128	-3.420560
6	-12.317767	1.958159	3.961153
6	-12.458028	0.622757	4.321141
6	-12.540468	0.409270	-4.338015
6	-12.665021	1.740927	-3.968396
6	-12.772640	-2.289737	3.598517

6	-12.915967	-3.262967	2.623829
6	-12.950796	3.877479	-1.858911
6	-13.075433	4.251854	-0.537603
6	-13.218423	-4.116247	-0.251177
6	-13.341789	-3.799268	-1.586207
1	14.335270	3.734010	-2.049915
1	14.121023	4.306750	0.345025
1	14.069381	-4.429097	-0.105230
1	13.853043	-3.761105	-2.474452
1	13.923033	3.608778	2.360126
1	13.669243	1.882915	4.085408
1	13.665480	-2.188341	-3.921597
1	13.446622	0.165871	-4.571922
1	13.464449	-0.225137	4.501542
1	13.218317	-2.579735	3.864681
1	13.295061	2.115681	-3.717823
1	13.046131	-3.836524	2.147889
1	-13.046141	3.835835	2.149036
1	-13.295052	-2.114574	-3.718488
1	-13.218320	2.578554	3.865433
1	-13.464453	0.223765	4.501585
1	-13.446624	-0.164478	-4.571953
1	-13.665482	2.189536	-3.920909
1	-13.669243	-1.884163	4.084840
1	-13.923033	-3.609508	2.359040
1	-13.853039	3.761875	-2.473317
1	-14.069377	4.429144	-0.103892
1	-14.121025	-4.306856	0.343720
1	-14.335269	-3.733387	-2.051048

Nanotube (7,5) u10v10
B3LYP/STO-3G Energy: -9802.389033

6	-13.431066	-3.332256	-2.475798
6	-13.299115	-3.980466	-1.267655
6	-13.207189	4.183624	0.599714
6	-13.086546	4.161621	-0.773484
6	-12.987566	-3.891306	1.728950
6	-12.845345	-3.199379	2.919624
6	-12.798489	2.638429	-3.360329
6	-12.667944	1.446979	-4.058821
6	-12.545124	-0.566736	4.362323
6	-12.414692	0.816936	4.356163
6	-12.394661	-1.533354	-3.900873
6	-12.273687	-2.711790	-3.110953
6	-12.154961	3.318939	2.719051
6	-12.044165	3.954288	1.447326
6	-12.003576	-4.100151	-0.612217
6	-11.857688	-4.091781	0.844907
6	-11.797981	3.947336	-1.414766
6	-11.664334	3.231117	-2.688468
6	-11.559991	-2.682626	3.334111
6	-11.416277	-1.416871	4.073809
6	-11.393955	0.778589	-4.162906
6	-11.268121	-0.700689	-4.145093
6	-11.145785	1.445359	4.095097
6	-11.025408	2.717831	3.335137
6	-10.966966	-3.128252	-2.660811
6	-10.834462	-3.854071	-1.411801
6	-10.742807	4.092637	0.839818
6	-10.622501	4.114526	-0.605444
6	-10.547124	-3.910841	1.411992
6	-10.399176	-3.221569	2.680714
6	-10.359514	2.782725	-3.099879
6	-10.224997	1.557464	-3.865117
6	-10.111973	-0.821372	4.176386
6	-9.975385	0.621386	4.216111
6	-9.946505	-1.269639	-3.947829

6	-9.799853	-2.520291	-3.251229
6	-9.706317	3.111041	2.869244
6	-9.568823	3.852333	1.643783
6	-9.510610	-4.023261	-0.840599
6	-9.365775	-4.092606	0.583101
6	-9.302942	3.978892	-1.197308
6	-9.170533	3.341510	-2.474364
6	-9.070796	-2.810514	3.109865
6	-8.926600	-1.621621	3.898684
6	-8.897290	0.980999	-4.045223
6	-8.761154	-0.447634	-4.136589
6	-8.648250	1.208922	4.070014
6	-8.516525	2.492688	3.433062
6	-8.477782	-2.977224	-2.853249
6	-8.337235	-3.774237	-1.657178
6	-8.251662	4.053391	1.061917
6	-8.123500	4.158870	-0.374136
6	-8.045938	-3.992481	1.171542
6	-7.899691	-3.377171	2.475092
6	-7.857896	2.960116	-2.948237
6	-7.724520	1.779225	-3.781447
6	-7.613433	-1.055751	4.103334
6	-7.476375	0.385275	4.231319
6	-7.450248	-1.045437	-4.032935
6	-7.309571	-2.353375	-3.418902
6	-7.209292	2.957566	3.034247
6	-7.077539	3.788370	1.850943
6	-7.025266	-3.991318	-1.098322
6	-6.880508	-4.139230	0.335947
6	-6.817120	4.068677	-0.978552
6	-6.685705	3.492456	-2.300765
6	-6.588764	-2.997867	2.936312
6	-6.445368	-1.840971	3.793617
6	-6.414513	1.214276	-3.999757
6	-6.277150	-0.213553	-4.166630
6	-6.166292	0.981334	4.123775
6	-6.031715	2.300908	3.554237
6	-5.995482	-2.822982	-3.039348
6	-5.852739	-3.684004	-1.891249
6	-5.766994	4.007114	1.277628
6	-5.636386	4.189493	-0.146915
6	-5.560635	-4.053460	0.928412
6	-5.414282	-3.514889	2.257402
6	-5.369804	3.123041	-2.785825
6	-5.234871	1.997117	-3.677066
6	-5.125864	-1.280635	4.016163
6	-4.986503	0.140168	4.225191
6	-4.959299	-0.815662	-4.091339
6	-4.818975	-2.152477	-3.561822
6	-4.716276	2.784337	3.178529
6	-4.584438	3.682285	2.053014
6	-4.533669	-3.927170	-1.341285
6	-4.388397	-4.155059	0.080990
6	-4.323551	4.128509	-0.756784
6	-4.192129	3.625228	-2.109245
6	-4.097568	-3.162858	2.743065
6	-3.954346	-2.054605	3.667721
6	-3.923554	1.446025	-3.933924
6	-3.786910	0.024014	-4.184954
6	-3.675859	0.743485	4.159744
6	-3.541062	2.101190	3.666557
6	-3.507492	-2.646547	-3.215852
6	-3.364970	-3.578916	-2.114704
6	-3.277574	3.937056	1.495851
6	-3.147351	4.203127	0.077084
6	-3.075209	-4.105299	0.677134
6	-2.929642	-3.639076	2.040241
6	-2.883773	3.282986	-2.613869
6	-2.749632	2.204570	-3.568274
6	-2.642699	-1.508388	3.920168

6	-2.502633	-0.099107	4.209102
6	-2.475398	-0.579715	-4.141700
6	-2.334882	-1.944179	-3.690758
6	-2.230776	2.600401	3.316143
6	-2.097736	3.560018	2.246028
6	-2.048332	-3.844331	-1.576478
6	-1.902423	-4.150736	-0.174185
6	-1.835090	4.166172	-0.533986
6	-1.702980	3.740850	-1.906510
6	-1.610834	-3.308472	2.540584
6	-1.466932	-2.260169	3.521795
6	-1.434748	1.666059	-3.851909
6	-1.297722	0.267292	-4.183662
6	-1.186654	0.506422	4.174961
6	-1.050406	1.884879	3.763994
6	-1.017477	-2.457052	-3.373569
6	-0.874167	-3.450305	-2.332025
6	-0.784697	3.846093	1.704885
6	-0.653745	4.194181	0.305962
6	-0.584144	-4.137673	0.424605
6	-0.438792	-3.750420	1.813015
6	-0.391645	3.431043	-2.433181
6	-0.258641	2.406844	-3.450208
6	-0.153063	-1.732764	3.812596
6	-0.013293	-0.338383	4.184471
6	0.013290	-0.338220	-4.184502
6	0.153061	-1.732616	-3.812686
6	0.258639	2.406712	3.450293
6	0.391645	3.430950	2.433306
6	0.438794	-3.750351	-1.813187
6	0.584147	-4.137655	-0.424791
6	0.653747	4.194191	-0.305808
6	0.784699	3.846156	-1.704745
6	0.874166	-3.450393	2.331866
6	1.017474	-2.457182	3.373450
6	1.050405	1.885024	-3.763932
6	1.186653	0.506585	-4.174959
6	1.297717	0.267129	4.183659
6	1.434744	1.665909	3.851965
6	1.466933	-2.260031	-3.521907
6	1.610836	-3.308372	-2.540738
6	1.702981	3.740776	1.906647
6	1.835092	4.166148	0.534140
6	1.902425	-4.150738	0.174000
6	2.048332	-3.844386	1.576305
6	2.097738	3.560101	-2.245898
6	2.230778	2.600528	-3.316053
6	2.334877	-1.944321	3.690665
6	2.475391	-0.579877	4.141666
6	2.502634	-0.098942	-4.209126
6	2.642702	-1.508234	-3.920251
6	2.749628	2.204432	3.568355
6	2.883771	3.282884	2.613992
6	2.929646	-3.638993	-2.040404
6	3.075213	-4.105266	-0.677315
6	3.147353	4.203124	-0.076927
6	3.277576	3.937108	-1.495705
6	3.364968	-3.578992	2.114545
6	3.507486	-2.646670	3.215733
6	3.541065	2.101332	-3.666487
6	3.675861	0.743649	-4.159733
6	3.786901	0.023850	4.184952
6	3.923547	1.445872	3.933980
6	3.954351	-2.054461	-3.667823
6	4.097573	-3.162747	-2.743208
6	4.192128	3.625142	2.109382
6	4.323553	4.128472	0.756939
6	4.388399	-4.155046	-0.081169
6	4.533668	-3.927213	1.341115
6	4.584442	3.682358	-2.052876

6	4.716280	2.784459	-3.178430
6	4.818966	-2.152614	3.561731
6	4.959289	-0.815823	4.091306
6	4.986508	0.140335	-4.225205
6	5.125871	-1.280476	-4.016233
6	5.234864	1.996973	3.677146
6	5.369801	3.122928	2.785947
6	5.414288	-3.514794	-2.257554
6	5.560639	-4.053413	-0.928583
6	5.636389	4.189476	0.147076
6	5.766998	4.007154	-1.277474
6	5.852734	-3.684069	1.891095
6	5.995474	-2.823098	3.039233
6	6.031720	2.301046	-3.554157
6	6.166298	0.981497	-4.123753
6	6.277138	-0.213718	4.166631
6	6.414502	1.214118	3.999814
6	6.445376	-1.840819	-3.793705
6	6.588773	-2.997746	-2.936441
6	6.685703	3.492357	2.300904
6	6.817122	4.068625	0.978711
6	6.880512	-4.139202	-0.336115
6	7.025265	-3.991348	1.098159
6	7.077544	3.788432	-1.850795
6	7.209297	2.957681	-3.034136
6	7.309559	-2.353508	3.418815
6	7.450235	-1.045598	4.032907
6	7.476382	0.385444	-4.231319
6	7.613442	-1.055588	-4.103389
6	7.724510	1.779073	3.781531
6	7.857890	2.959993	2.948361
6	7.899700	-3.377062	-2.475228
6	8.045945	-3.992418	-1.171699
6	8.123503	4.158837	0.374302
6	8.251667	4.053417	-1.061755
6	8.337231	-3.774289	1.657031
6	8.477772	-2.977331	2.853140
6	8.516531	2.492823	-3.432970
6	8.648257	1.209085	-4.069978
6	8.761139	-0.447800	4.136594
6	8.897277	0.980836	4.045284
6	8.926610	-1.621462	-3.898755
6	9.070807	-2.810382	-3.109976
6	9.170530	3.341397	2.474504
6	9.302943	3.978823	1.197471
6	9.365780	-4.092561	-0.583255
6	9.510609	-4.023275	0.840448
6	9.568828	3.852383	-1.643625
6	9.706323	3.111150	-2.869121
6	9.799840	-2.520417	3.251149
6	9.946489	-1.269798	3.947807
6	9.975394	0.621556	-4.216096
6	10.111984	-0.821203	-4.176425
6	10.224986	1.557305	3.865206
6	10.359507	2.782589	3.100005
6	10.399187	-3.221446	-2.680832
6	10.547134	-3.910761	-1.412132
6	10.622505	4.114473	0.605615
6	10.742813	4.092647	-0.839646
6	10.834458	-3.854108	1.411665
6	10.966956	-3.128350	2.660709
6	11.025415	2.717963	-3.335031
6	11.145792	1.445525	-4.095048
6	11.268105	-0.700858	4.145109
6	11.393941	0.778418	4.162977
6	11.416288	-1.416702	-4.073868
6	11.560005	-2.682480	-3.334206
6	11.664330	3.230990	2.688614
6	11.797983	3.947249	1.414935
6	11.857697	-4.091713	-0.845046

6	12.003577	-4.100149	0.612078
6	12.044172	3.954322	-1.447158
6	12.154967	3.319040	-2.718916
6	12.273674	-2.711914	3.110885
6	12.394642	-1.533521	3.900875
6	12.414700	0.817115	-4.356139
6	12.545133	-0.566557	-4.362351
6	12.667930	1.446813	4.058927
6	12.798480	2.638283	3.360469
6	12.845359	-3.199232	-2.919726
6	12.987578	-3.891195	-1.729071
6	13.086548	4.161551	0.773664
6	13.207194	4.183612	-0.599533
6	13.299112	-3.980498	1.267532
6	13.431056	-3.332352	2.475710
1	-14.427145	-3.156405	-2.905164
1	-14.197367	-4.324530	-0.738875
1	-14.199985	4.237667	1.067567
1	-13.990800	4.202153	-1.394451
1	-13.993704	-4.166512	1.387642
1	-13.741778	-2.938923	3.497091
1	-13.801341	3.053174	-3.196114
1	-13.571670	0.945990	-4.429339
1	-13.548258	-1.006005	4.437145
1	-13.319239	1.434991	4.425341
1	-13.404913	-1.155725	-4.103154
1	-13.162653	3.091686	3.089120
1	13.162653	3.091815	-3.089001
1	13.404868	-1.155935	4.103230
1	13.319246	1.435174	-4.425293
1	13.548270	-1.005825	-4.437195
1	13.571653	0.945815	4.429441
1	13.801328	3.053038	3.196287
1	13.741796	-2.938749	-3.497176
1	13.993707	-4.166397	-1.387767
1	13.990803	4.202050	1.394634
1	14.199993	4.237669	-1.067379
1	14.197367	-4.324536	0.738741
1	14.427130	-3.156532	2.905095

Nanotube (7,5) u10v11
B3LYP/STO-3G Energy: -9877.686189

6	-13.534389	-2.529526	-3.294239
6	-13.412889	-3.466351	-2.292206
6	-13.297984	3.941669	1.603759
6	-13.168517	4.272648	0.272008
6	-13.119473	-4.151851	0.628480
6	-12.981562	-3.790007	1.957300
6	-12.869871	3.464703	-2.618194
6	-12.739951	2.491764	-3.597961
6	-12.679073	-1.617535	4.028424
6	-12.542890	-0.279503	4.377238
6	-12.480953	-0.431684	-4.205688
6	-12.370163	-1.773234	-3.743291
6	-12.262696	2.556343	3.435575
6	-12.141166	3.495577	2.370309
6	-12.121692	-3.757603	-1.682627
6	-11.984748	-4.124580	-0.272195
6	-11.876299	4.223139	-0.396217
6	-11.737324	3.857956	-1.809983
6	-11.696149	-3.404169	2.496930
6	-11.551654	-2.371795	3.536957
6	-11.467859	1.864212	-3.862699
6	-11.348739	0.429339	-4.223320
6	-11.269374	0.387878	4.291808
6	-11.139075	1.811383	3.883499
6	-11.067935	-2.299109	-3.408615

6	-10.946460	-3.321780	-2.386876
6	-10.835150	3.778565	1.825708
6	-10.705404	4.170531	0.435189
6	-10.676834	-4.103603	0.328897
6	-10.533643	-3.764325	1.732973
6	-10.431739	3.522941	-2.316120
6	-10.297588	2.534054	-3.369489
6	-10.245537	-1.829954	3.795532
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6	-10.031230	-0.179070	-4.171842
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6	-9.244687	3.895066	-1.561769
6	-9.206287	-3.484426	2.259662
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6	-8.772834	0.151947	4.219507
6	-8.631905	1.554707	3.933361
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6	-8.447489	-3.196154	-2.591315
6	-8.345591	3.669770	2.042954
6	-8.207639	4.139515	0.683350
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6	-8.033327	-3.875712	1.506129
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6	-2.820826	3.038345	-2.876899
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6	-2.555797	0.492994	-4.144341
6	-2.424737	-0.942674	-4.058663
6	-2.344989	1.654968	3.881136
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6	-1.744160	-3.860698	1.617124
6	-1.601418	-3.099418	2.834284
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6	0.742173	-3.958156	1.389711
6	0.883747	-3.264533	2.651470
6	0.979662	2.755317	-3.126113
6	1.111859	1.527605	-3.877500
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6	1.313853	0.595180	4.177196
6	1.373992	-1.315371	-3.960097
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