

Electronic Supplementary Information  
to

**Unraveling origins of the heterogeneous curvature  
dependence of polypeptide interactions with carbon  
nanostructures: a computational study**

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  - 1 and 2 contributed equally

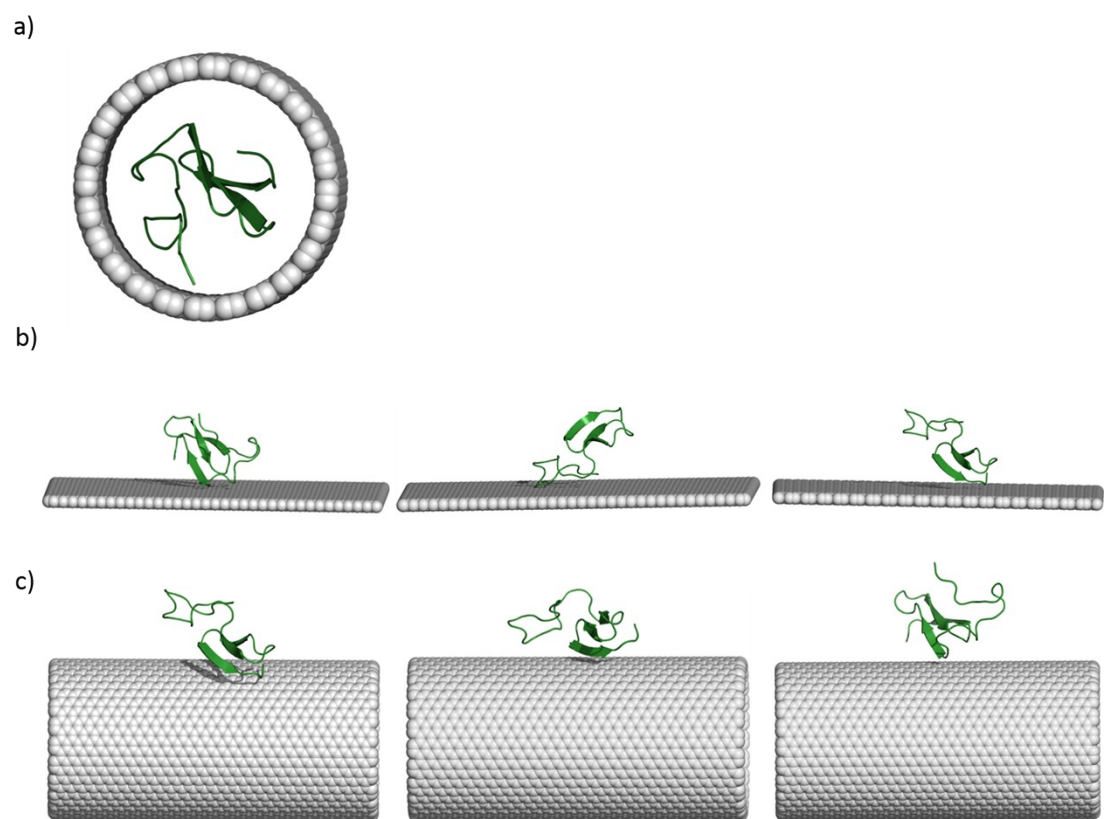


Figure S1. Snapshots of starting conformations of peptide nanosurface MD simulations, for peptide on the a) concave surface; b) planar surface; c) concave surface. The water molecules are not shown for clarity.

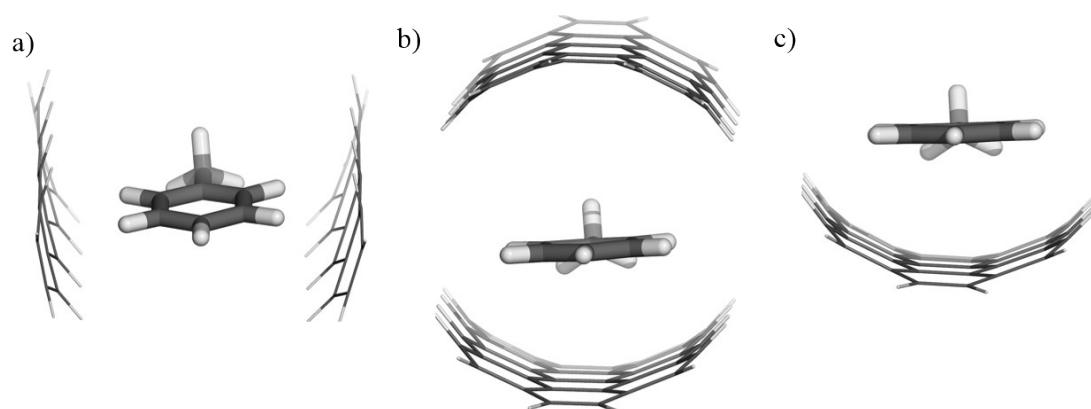


Figure S2: A schematic representation of interaction of a) toluene with the sidewalls of concave surface of SWCNT where hydrogens of phenyl ring and methyl group are interacting through CH- $\pi$ , b) toluene with lower and upper wall and c) toluene with lower wall of concave surface of SWCNT through  $\pi$ - $\pi$  of phenyl ring and CH- $\pi$  of hydrogens of methyl substituent. Atom Colors: grey-carbon and white-hydrogen.

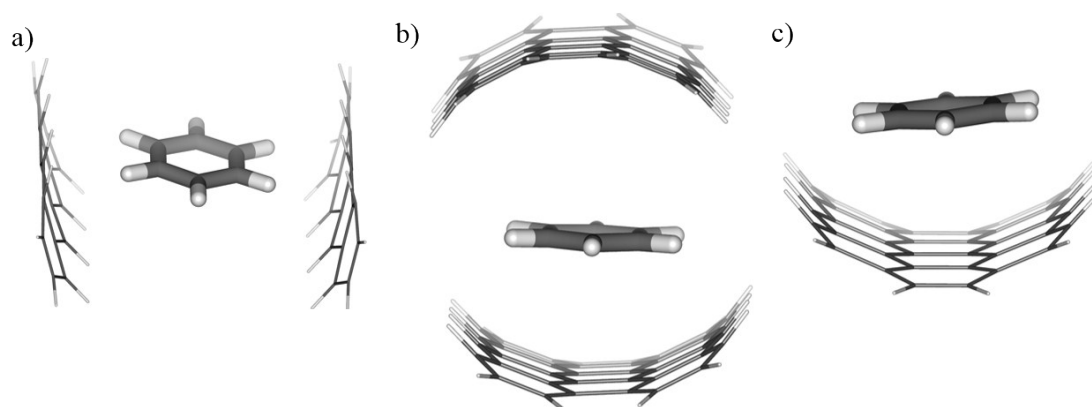


Figure S3: A schematic representation of interaction of a) benzene with the sidewalls of concave surface of SWCNT where hydrogens of phenyl ring are interacting through CH- $\pi$ , b) benzene with lower and upper wall and c) benzene with lower wall of concave surface of SWCNT through  $\pi$ - $\pi$  of phenyl ring. Atom Colors: grey-carbon and white-hydrogen.

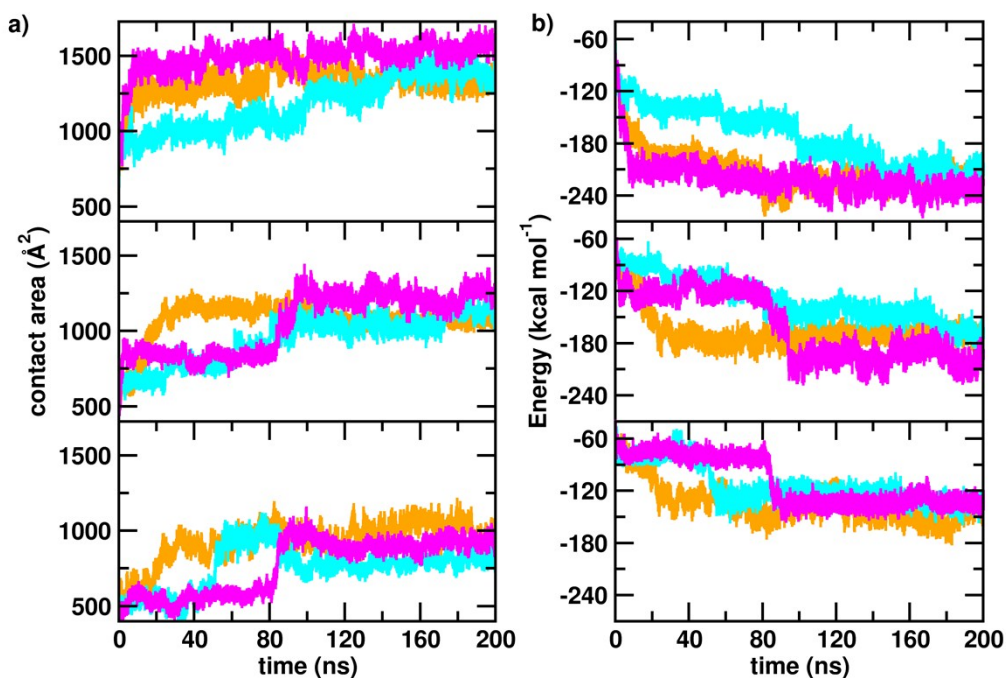


Figure S4: Time evolution of a) total peptide-SWCNT contact area, and b) total peptide-SWCNT interaction energy along the three independent simulation trajectories. The upper, middle and lower panels represent the systems corresponding to the concave, planar and convex surfaces, respectively.

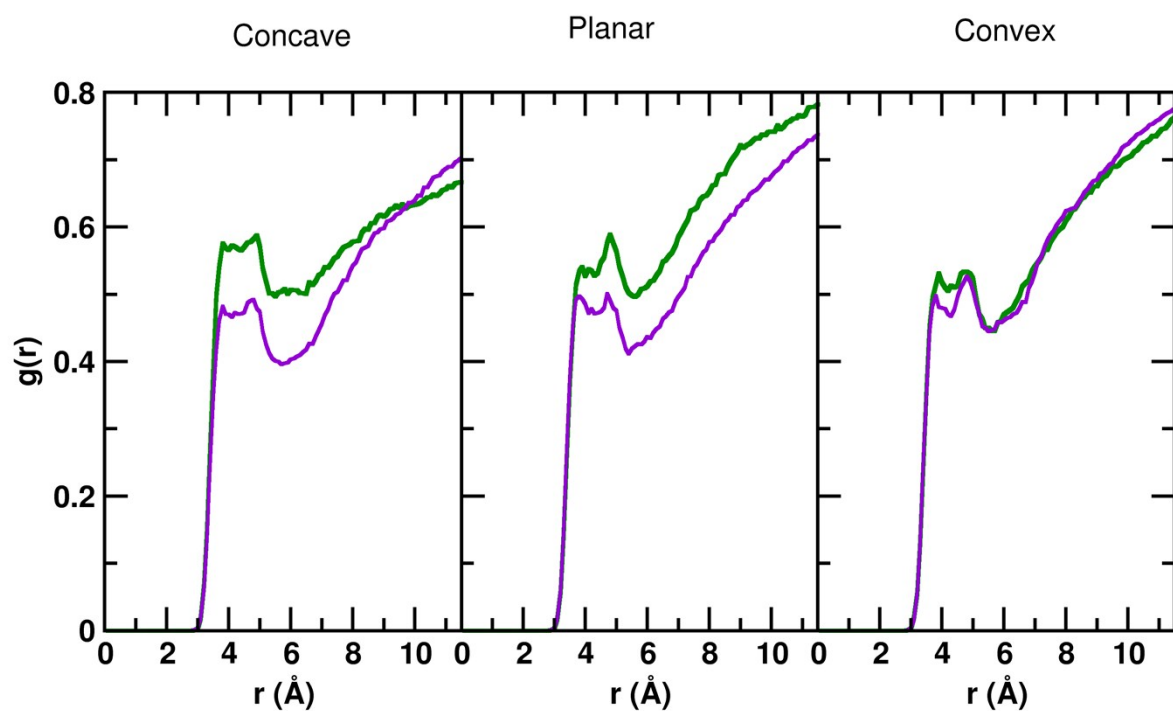


Figure S5: Protein  $C_\beta$  atom-water oxygen radial distribution functions before (*in green*) and after (*in purple*) peptide adsorption on the individual carbon nanosurfaces. Each data set is calculated using snapshots from a cumulative simulation time of 30 ns.

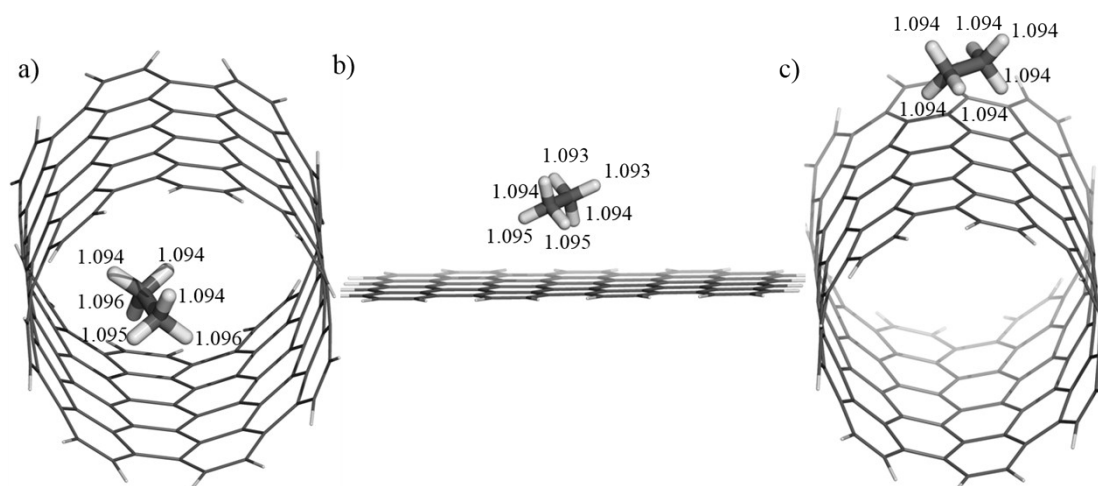


Figure S6: The gas phase optimized geometries of ethane with concave surface of SWCNT, graphene and convex surface of SWCNT at the M062X/6-31G\*\* level of theory. The values correspond to the C-H bond distances of ethane. All the values are in Å. Atom Colors: grey-carbon and white-hydrogen.

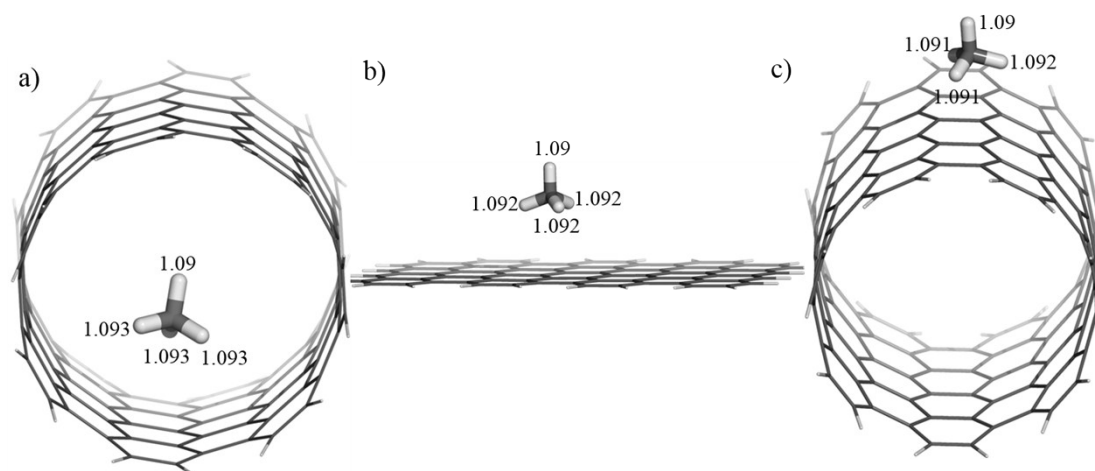


Figure S7: The gas phase optimized geometries of methane with concave surface of SWCNT, graphene and convex surface of SWCNT at the M062X/6-31G\*\* level of theory. The values correspond to the C-H bond distances of methane. All the values are in Å. Atom Colors: grey-carbon and white-hydrogen.



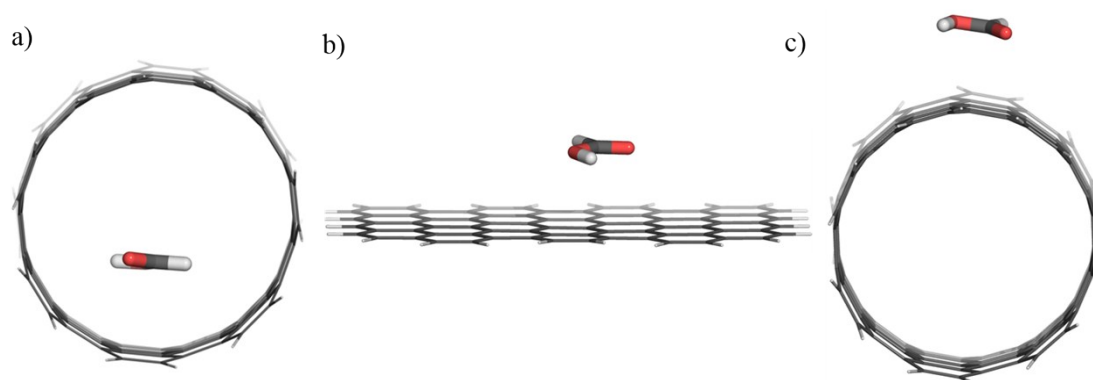


Figure S8: The gas phase optimized geometries of formic acid with a) concave surface of SWCNT, b) graphene and c) convex surface of SWCNT at the M062X/6-31G\*\* level of theory. Atom Colors: grey-carbon, white-hydrogen and red-oxygen.

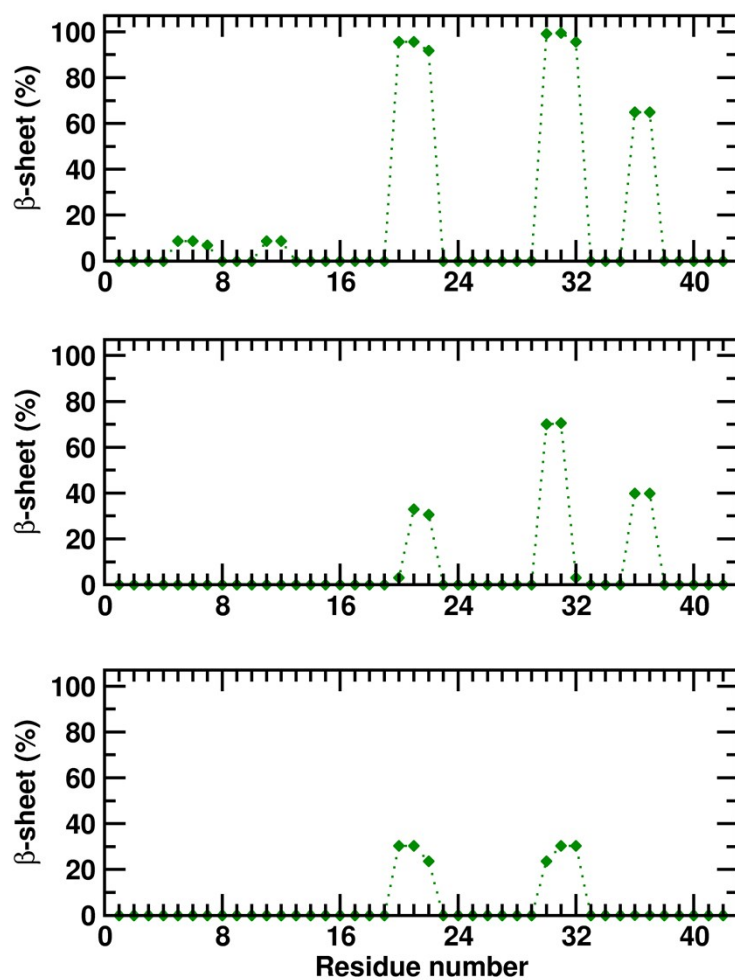


Figure S9: The residue-wise secondary structure fractions of the peptides after adsorption, in the systems corresponding to the concave (top panel), planar (middle panel), and convex (lower panel) surfaces, respectively.

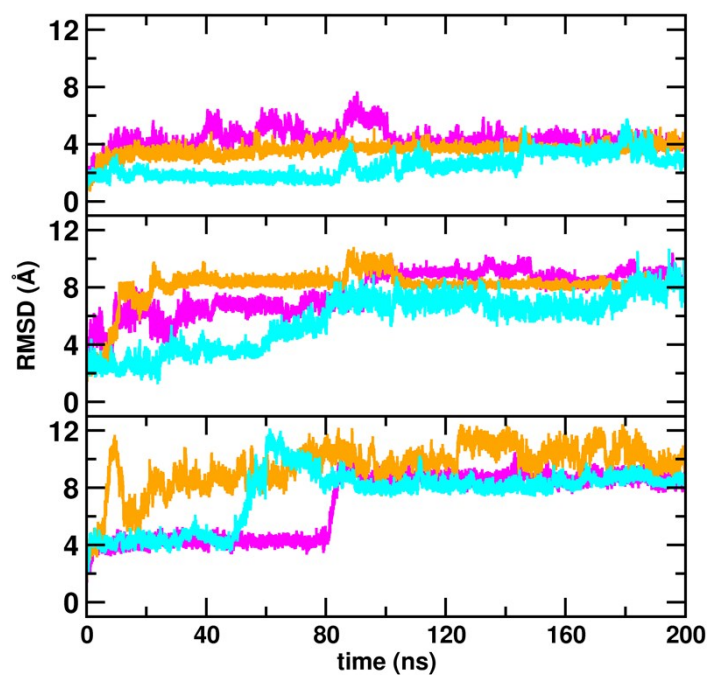


Figure S10: Time evolution of backbone RMSD of the peptide along the three independent simulation trajectories of each system. The upper, middle and lower panels represent the systems corresponding to the concave, planar and convex surfaces, respectively.

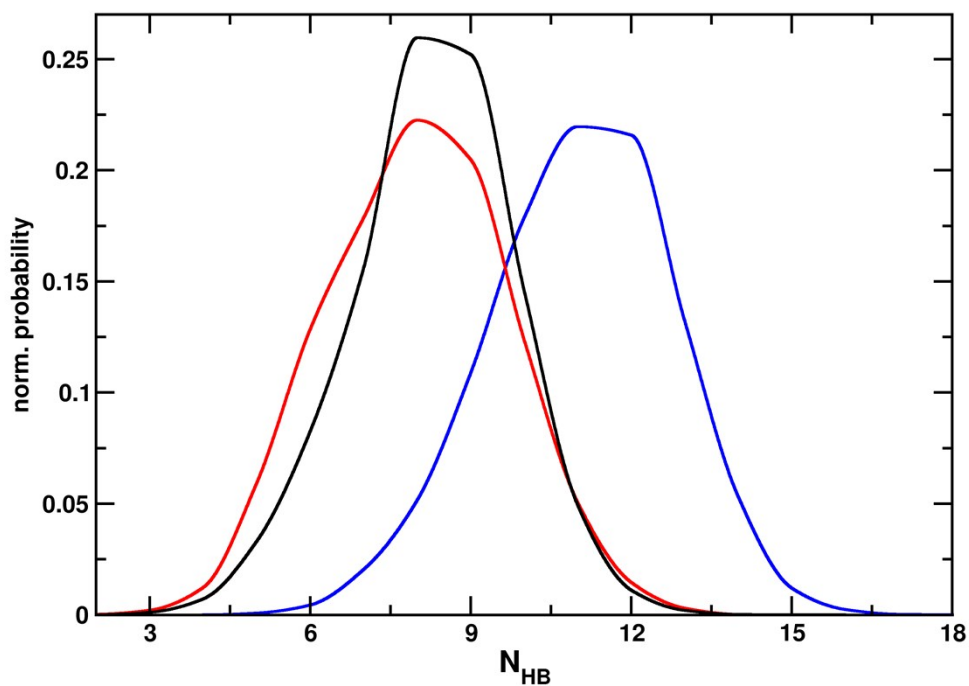


Figure S11: Normalized distributions of the number of intra-peptide backbone hydrogen bonds ( $N_{HB}$ ) of the peptide after adsorption on the surfaces, in the systems with concave (*in blue*), planar (*in black*) and convex (*in red*) surfaces. Data is obtained using the 120 ns of cumulative simulation time from the last parts of the simulation trajectories.

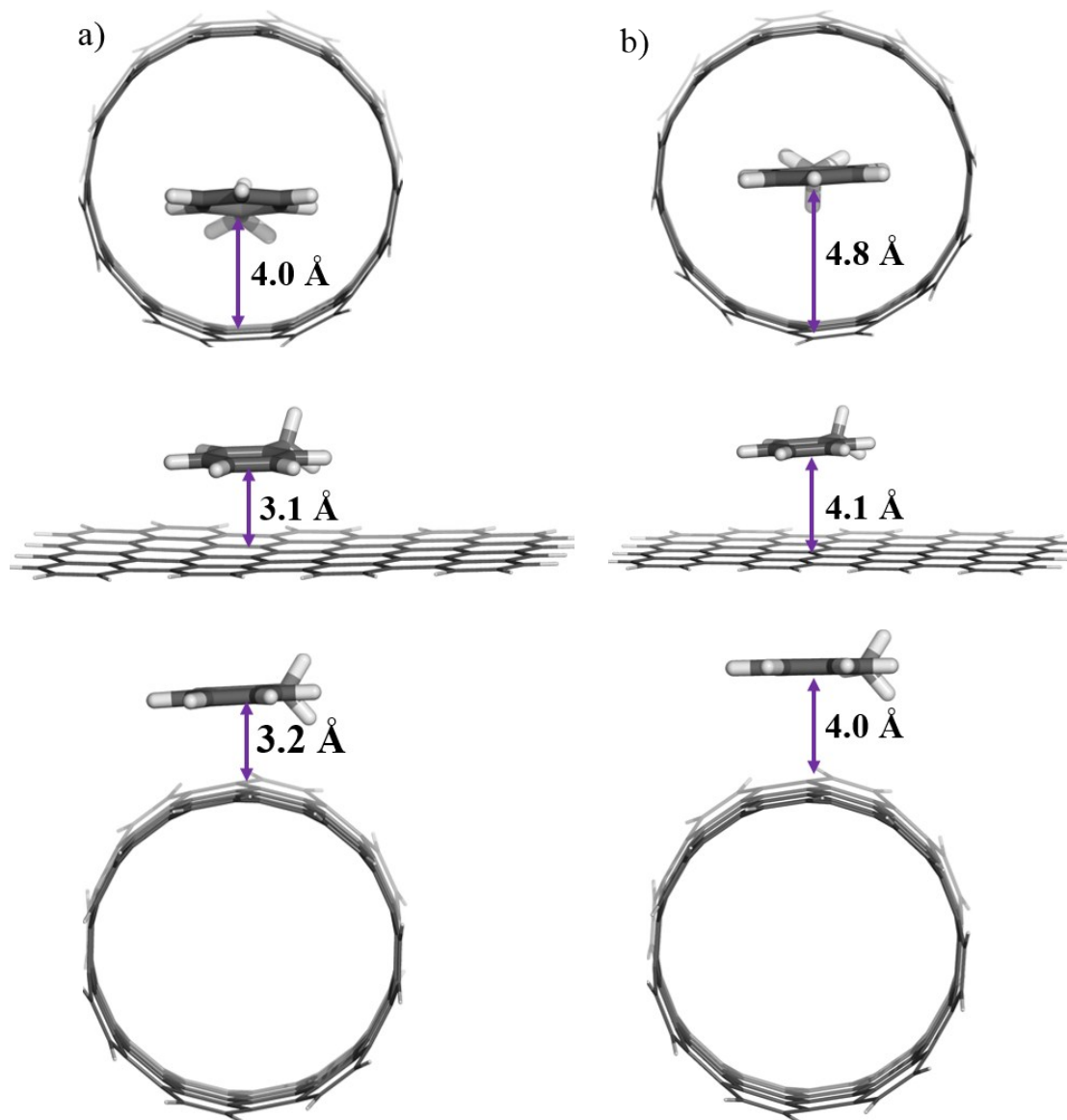


Figure S12: The gas phase optimized geometries of toluene with concave surface of SWCNT, graphene and convex surface of SWCNT at the a) dispersion corrected B3LYP-D2/6-31G\*\* and b) B3LYP/6-31G\*\* level of theories. The distances (Å) are calculated normal to the CNSs from the geometrical centers of toluene. Atom Colors: grey-carbon and white-hydrogen.

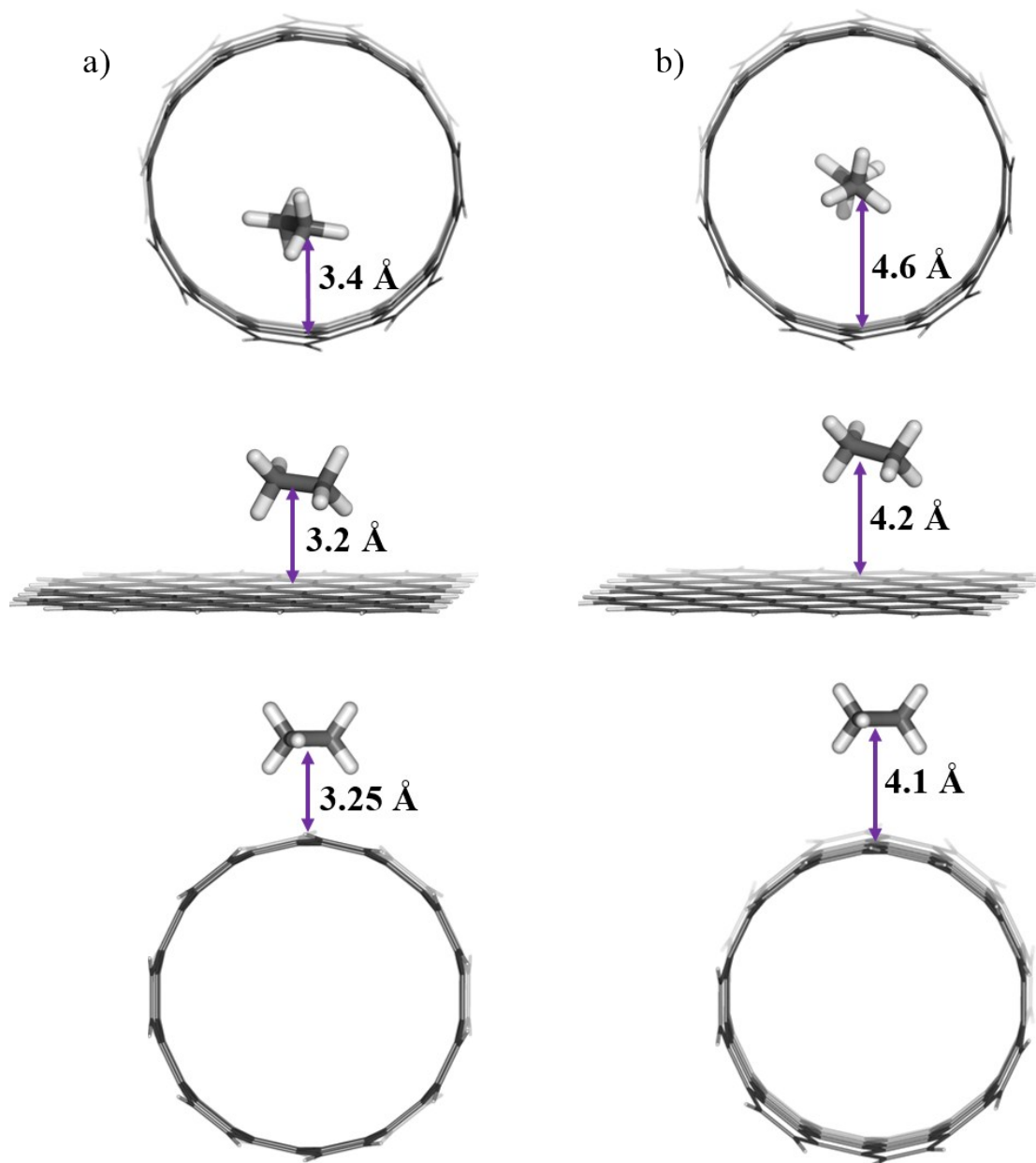


Figure S13: The gas phase optimized geometries of ethane with concave surface of SWCNT, graphene and convex surface of SWCNT at the a) dispersion corrected B3LYP-D2/6-31G\*\* and b) B3LYP/6-31G\*\* level of theories. The distances (Å) are calculated normal to the CNSs from the geometrical centers of ethane. Atom Colors: grey-carbon and white-hydrogen.

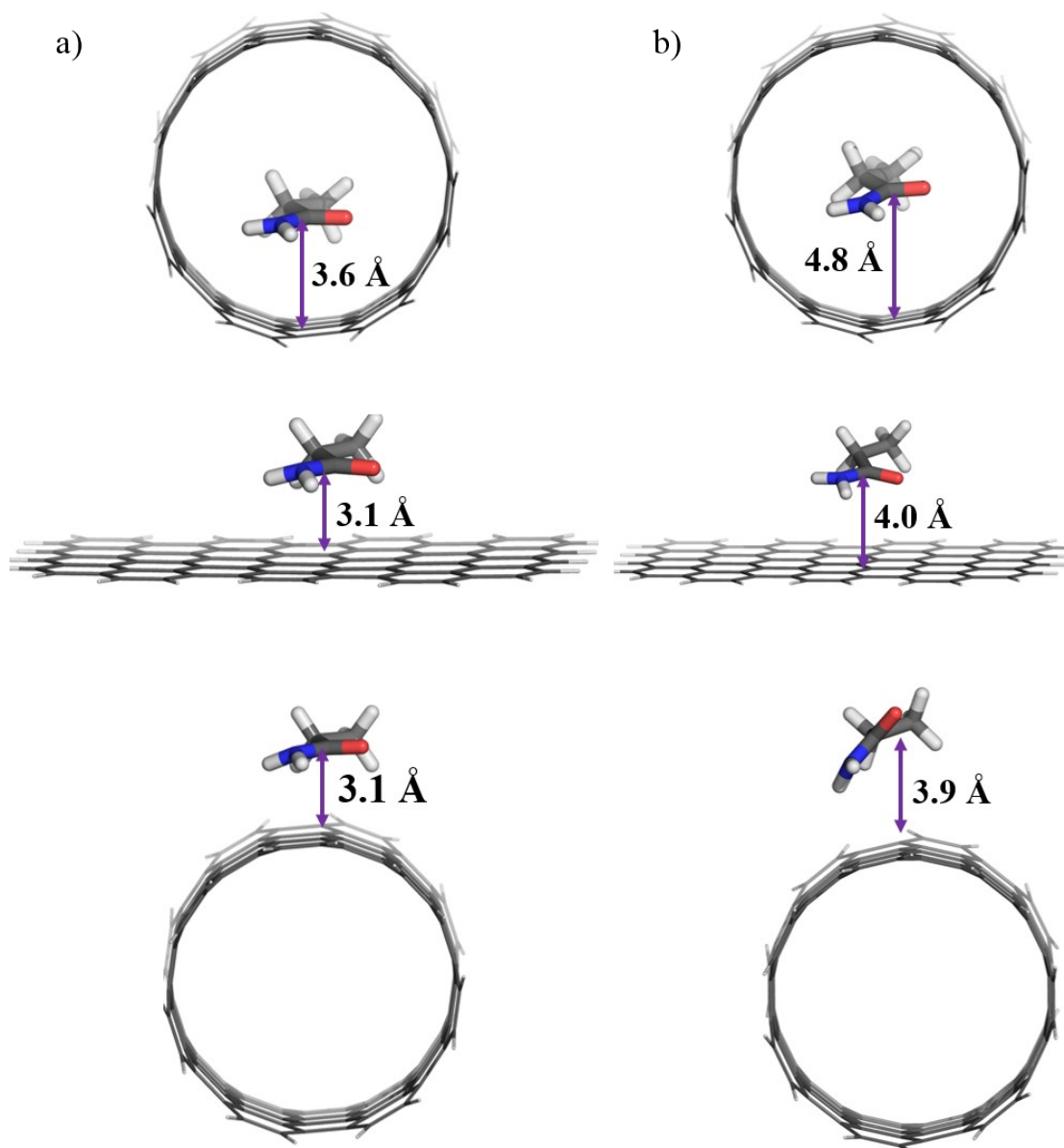


Figure S14: The gas phase optimized geometries of propanamide with concave surface of SWCNT, graphene and convex surface of SWCNT at the a) dispersion corrected B3LYP-D2/6-31G\*\* and b) B3LYP/6-31G\*\* level of theories. The distances (Å) are calculated normal to the CNSs from the geometrical centers of propanamide. Atom Colors: grey-carbon, white-hydrogen, red-oxygen and blue-nitrogen.

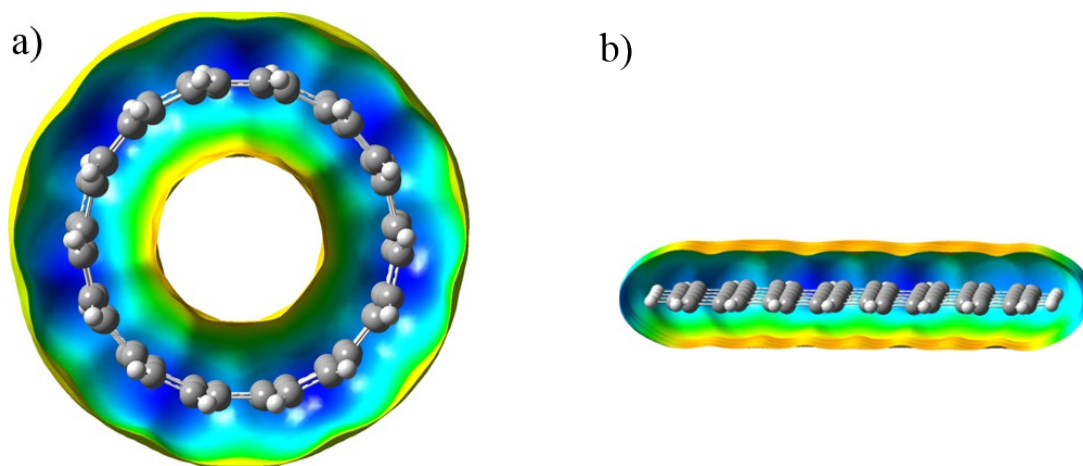


Figure S15: Molecular electrostatic potential isosurfaces of a) nanotube and b) graphene at the M062X/6-31G\*\* level of theory. The blue color indicates large positive potential, the red color indicates large negative potential, whereas yellow and green colors indicate intermediate values.



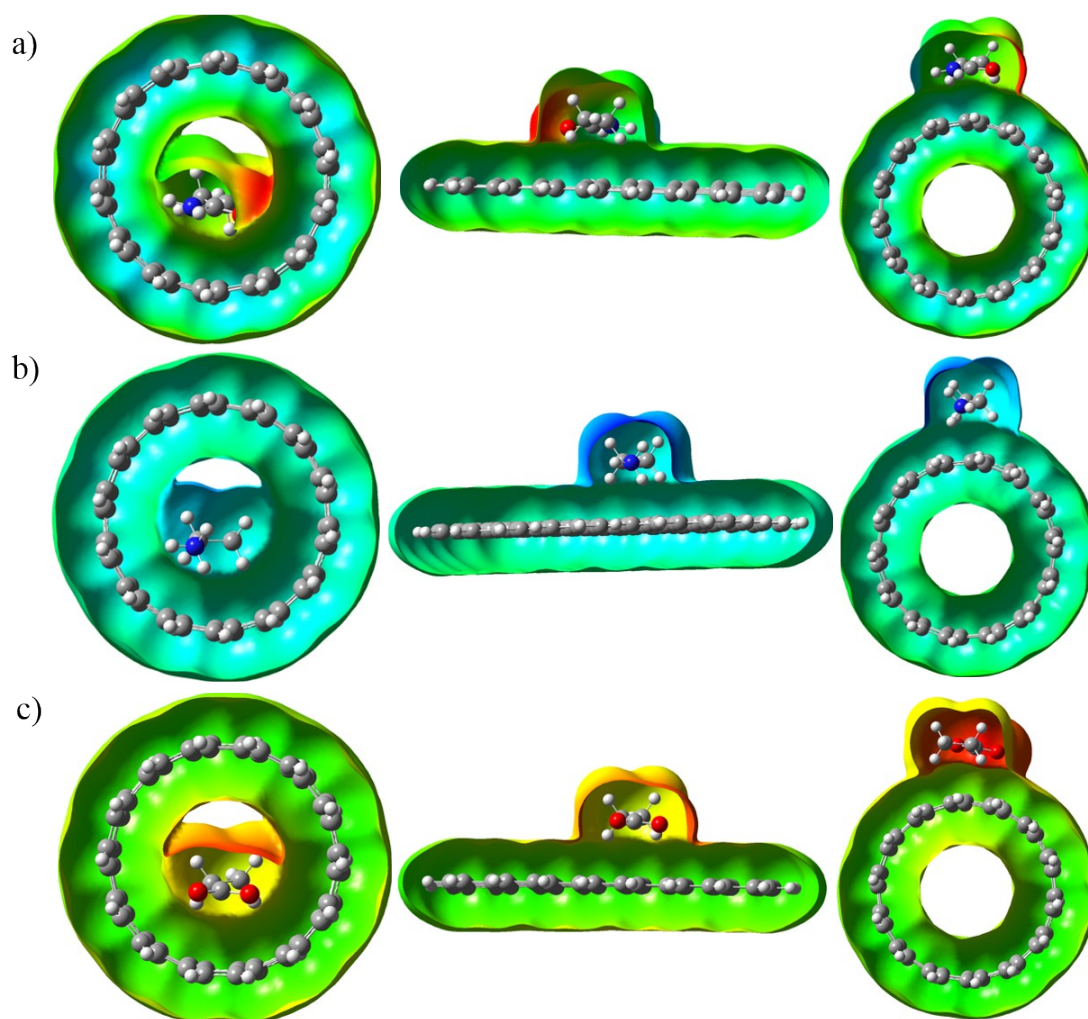


Figure S16: Molecular electrostatic potential isosurfaces of a) propanamide at the M062X/6-31G\*\* level of theory, and b) ethylammonium and c) propanoate at the CPCM/M062X/6-31G\*\* level of theory while in interaction with concave surface of SWCNT, graphene and convex surface of SWCNT respectively from left to right. The blue color indicates large positive potential, the red color indicates large negative potential, whereas yellow and green colors indicate intermediate values.

Table S1. Mean solvation number ( $W_i$ ) around protein 10 ns before adsorption; Mean solvation number ( $W_f$ ) around protein 10 ns after adsorption; standard deviations are provided within braces. The mean desolvation number,  $\Delta W$ , is the difference between  $W_i$  and  $W_f$ .

| System  | $W_i$        | $W_f$        | $\Delta W$ |
|---------|--------------|--------------|------------|
| Concave | 205.0 (10.4) | 163.4 (7.5)  | 41.6       |
| Planar  | 207.2 (9.7)  | 189.6 (8.3)  | 17.6       |
| Convex  | 211.5 (12.1) | 199.5 (10.2) | 12.0       |

Table S2. The interaction energies in kcal mol<sup>-1</sup> of toluene and benzene with different walls of concave surface of SWCNT at the M062X/6-31G\*\* level of theory in gas phase

| E <sub>i</sub> | total <sup>a</sup> | Lower wall <sup>b</sup> | (Lower + upper) walls <sup>c</sup> | Side-walls <sup>d</sup> | Sum <sup>e</sup> |
|----------------|--------------------|-------------------------|------------------------------------|-------------------------|------------------|
| Toluene        | -19.7              | -12.0                   | -12.2                              | -5.4                    | -17.4            |
| Benzene        | -16.2              | -8.9                    | -9.3                               | 7.0                     | -15.9            |

- a) Net interaction energy arises due to all the surfaces of concave surface of SWCNT
- b) Interaction energy only due to lower wall of SWCNT
- c) Interaction energy due to upper and lower walls of SWCNT
- d) Interaction energy due to both the side walls of SWCNT
- e) Sum of interaction energies with lower and two side walls of concave surface of SWCNT

Table S3. The C-O and C-N bond distances (in Å) in the amido group of propanamide and C-O bond distances (in Å) in the carboxylic group of propanoic acid at the M062X/6-31G\*\* level of theory.

|                |    | Concave |         | Planar |         | Convex |         | Free  |         |
|----------------|----|---------|---------|--------|---------|--------|---------|-------|---------|
|                |    | Gas     | Solvent | Gas    | solvent | Gas    | Solvent | gas   | Solvent |
| Propanamide    | 1  | 1.221   | 1.225   | 1.218  | 1.225   | 1.216  | 1.225   | 1.236 | 1.225   |
|                | 2  | 1.36    | 1.356   | 1.37   | 1.359   | 1.369  | 1.356   | 1.368 | 1.354   |
| Propanoic acid | 1' | 1.208   | 1.21    | 1.207  | 1.21    | 1.206  | 1.21    | 1.22  | 1.209   |
|                | 2' | 1.347   | 1.345   | 1.348  | 1.345   | 1.348  | 1.343   | 1.4   | 1.343   |

1, 2, 1', 2' represent covalent bond lengths as shown in following figure in optimized geometries of a) propanamide and b) propanoic acid respectively

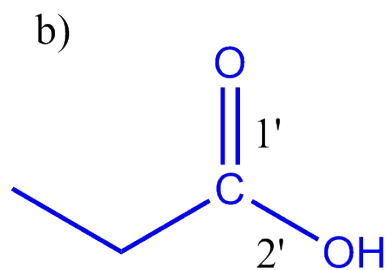
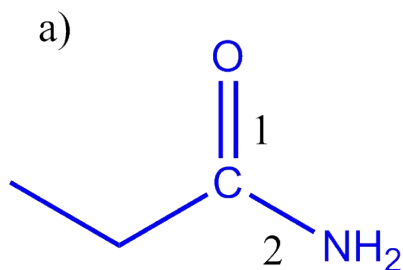


Table S4. The Mulliken charges on all the atoms of amido group of propanamide and carboxylic group of propanoic acid at the M062X/6-31G\*\* level of theory

|                |    | Concave |         | Planar |         | Convex |         | Free  |         |
|----------------|----|---------|---------|--------|---------|--------|---------|-------|---------|
|                |    | Gas     | Solvent | Gas    | solvent | Gas    | solvent | gas   | Solvent |
| Propanamide    | N  | -0.65   | -0.65   | -0.65  | -0.66   | -0.66  | -0.66   | -0.68 | -0.67   |
|                | C' | 0.59    | 0.58    | 0.57   | 0.58    | 0.58   | 0.58    | 0.59  | 0.59    |
|                | O' | -0.53   | -0.56   | -0.51  | -0.57   | -0.51  | -0.58   | -0.51 | -0.58   |
|                | H  | 0.28    | 0.29    | 0.29   | 0.31    | 0.29   | 0.32    | 0.29  | 0.32    |
|                | H  | 0.30    | 0.31    | 0.29   | 0.30    | 0.29   | 0.31    | 0.30  | 0.31    |
| Propanoic acid | O  | -0.48   | -0.50   | -0.48  | -0.51   | -0.48  | -0.52   | -0.47 | -0.52   |
|                | C' | 0.59    | 0.60    | 0.59   | 0.60    | 0.59   | 0.61    | 0.59  | 0.61    |
|                | O' | -0.51   | -0.52   | -0.52  | -0.53   | -0.52  | -0.52   | -0.53 | -0.53   |
|                | H  | 0.34    | 0.36    | 0.34   | 0.36    | 0.34   | 0.36    | 0.35  | 0.37    |

C' and O' represent carbonyl carbon and carbonyl oxygen (oxo) respectively.

Table S5. The interaction energies in kcal mol<sup>-1</sup> of ammonia with the different CNSs

| E <sub>i</sub> | Concave | Planar | Convex |
|----------------|---------|--------|--------|
| L <sub>1</sub> | -6.3    | -3.6   | -3.4   |
| L <sub>2</sub> | -7.7    | -5.1   | -4.8   |
| L <sub>3</sub> | -7.5    | -4.0   | -3.7   |
| L <sub>4</sub> | -4.5    | -2.9   | -2.8   |
| L <sub>5</sub> | -7.9    | -4.6   | -4.2   |
| L <sub>6</sub> | -5.6    | -3.4   | -3.1   |

L<sub>1</sub>, L<sub>2</sub>, L<sub>3</sub>, L<sub>4</sub>, L<sub>5</sub> and L<sub>6</sub> correspond the values at the gas/M062X/6-31G\*\*, gas/B3LYP-D2/6-31G\*\*, gas/M062X/6-311G\*\*, CPCM/M062X/6-311G\*\*, CPCM/B3LYP-D2/6-31G\*\* and CPCM/M062X/6-31G\*\* level of theories.

Table S6. The interaction energies in kcal mol<sup>-1</sup> of toluene, ethane and propanamide with the different CNSs

| E <sub>i</sub> | Toluene |        |        | Ethane  |        |        | Propanamide |        |        |
|----------------|---------|--------|--------|---------|--------|--------|-------------|--------|--------|
|                | Concave | Planar | Convex | Concave | Planar | Convex | Concave     | Planar | Convex |
| L <sub>2</sub> | -30.0   | -15.6  | -12.3  | -12.9   | -6.4   | -5.4   | -26.4       | -14.3  | -11.6  |
| L <sub>7</sub> | 2.6     | 0.0    | 0.0    | 0.1     | -0.1   | -0.2   | -2.0        | -1.1   | -1.6   |

L<sub>2</sub> and L<sub>7</sub> correspond the values at the gas/B3LYP-D2/6-31G\*\* and gas/B3LYP/6-31G\*\* level of theories.

Table S7. The difference in HOMO-LUMO energy gap in kcal mol<sup>-1</sup> of optimized geometries of AAA-CNS complexes and the HOMO-LUMO energy gap of corresponding bare CNSs at the M062X/6-31G\*\* level of theory

|               | Concave   | Planar      | Convex    |
|---------------|-----------|-------------|-----------|
| Toluene       | 0.1 (0.2) | -0.1 (-0.1) | 0.1 (0.1) |
| Ethane        | 0.1 (0.1) | 0.0 (0.1)   | 0.0 (0.1) |
| Propanamide   | 0.1 (0.3) | 0.0 (0.1)   | 0.0 (0.0) |
| Ethylammonium | 0.2       | 0.0         | 0.2       |
| Propanoate    | 0.3       | 0.1         | -0.1      |

Values outside the parenthesis are solvent phase and values inside the parenthesis are gas phase values. Ethylammonium-CNS and propanoate-CNS complexes are optimized only in solvent phase.

Table S8. The interaction energies of AAA with CNSs in kcal mol<sup>-1</sup>

| E <sub>i</sub> | Concave       | Planar        | Convex      |
|----------------|---------------|---------------|-------------|
| Toluene        | -21.6 (-21.7) | -11.6 (-11.8) | -8.8 (-8.8) |
| Ethane         | -9.4 (-9.7)   | -4.6 (-4.7)   | -3.6 (-3.6) |
| Propanamide    | -14.6 (-14.8) | -8.9 (-9.0)   | -7.3 (-7.3) |
| Ethylammonium  | -9.4 (-9.8)   | -5.9 (-6.1)   | -4.7 (-4.7) |
| Propanoate     | -11.2 (-11.4) | -6.0 (-6.0)   | -4.7 (-4.7) |

The values outside the parentheses are at the CPCM/M062X/6-31+G\*\* level of theory and value inside the parentheses are at the CPCM/M062X/6-31++G\*\* level of theory.

XYZ coordinates of all amino acid analogue-carbon nanosurface complexes after full optimization at the M062X/6-31G\*\* level of theory.

Toluene-concave surface of SWCNT, gas

|   |          |          |          |   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|---|----------|----------|----------|
| C | 5.48383  | 4.87610  | 1.12058  | C | -1.85016 | 2.04510  | 4.28249  | C | 4.29536  | -3.83212 | 2.99337  |
| C | 4.28760  | 4.56164  | 1.82533  | C | -1.85284 | 3.22503  | 3.52130  | C | 5.49187  | -4.33562 | 2.40936  |
| C | 3.07067  | 4.73386  | 1.13694  | C | -3.09714 | 3.73949  | 3.03093  | C | 5.49182  | -4.86348 | 1.14683  |
| C | 3.06982  | 4.87945  | -0.28734 | C | -4.31192 | 3.28367  | 3.58004  | C | 4.29456  | -4.92487 | 0.37854  |
| C | 4.28769  | 4.83654  | -0.99382 | C | -5.51451 | 4.57804  | 1.91078  | C | 4.29688  | -4.80996 | -1.06523 |
| C | 5.48421  | 5.00868  | -0.24133 | C | -5.51097 | 3.86450  | 3.07899  | C | 5.49714  | -4.61579 | -1.80573 |
| C | 1.82916  | 4.47610  | 1.80352  | C | -0.62010 | 3.73825  | 3.01892  | C | 5.49852  | -3.88390 | -2.96180 |
| C | 0.59350  | 4.71979  | 1.13278  | C | 0.60033  | 3.24399  | 3.51974  | C | 4.30047  | -3.29495 | -3.45644 |
| C | 0.59159  | 4.87009  | -0.28760 | C | 0.60357  | 2.04449  | 4.29270  | C | 4.30051  | -2.05747 | -4.20874 |
| C | 1.82759  | 4.76377  | -0.99469 | C | -0.61432 | 1.38150  | 4.54115  | C | 5.49725  | -1.35610 | -4.52408 |
| C | -0.62329 | 4.48734  | 1.80371  | C | -0.61301 | -0.03228 | 4.73458  | C | 5.49621  | 0.00100  | -4.70521 |
| C | -1.85955 | 4.69617  | 1.12387  | C | 0.60629  | -0.73528 | 4.67287  | C | 4.29852  | 0.75890  | -4.58273 |
| C | 1.86180  | 4.83629  | -0.27334 | C | 0.60539  | -2.09900 | 4.25403  | C | 4.29621  | 2.15326  | -4.19144 |
| C | -0.62765 | 4.77249  | -0.98874 | C | -0.61411 | -2.71378 | 3.90931  | C | 5.49286  | 2.86012  | -3.88508 |
| C | -3.10058 | 4.48675  | 1.81050  | C | -0.61592 | -3.77364 | 2.95406  | C | 5.49090  | 3.89396  | -2.98848 |
| C | -4.31916 | 4.76246  | 1.16074  | C | 0.60147  | -4.18610 | 2.37771  | C | 4.29074  | 4.29482  | -2.33653 |
| C | -4.32284 | 4.89258  | -0.28222 | C | 0.59977  | -4.74309 | 1.06365  | C | 1.35375  | 1.12160  | -0.87700 |
| C | -3.10702 | 4.74615  | -0.97813 | C | -0.61956 | -4.85977 | 0.36680  | C | 2.03650  | -0.08929 | -0.80853 |
| C | -3.10569 | 4.21460  | -2.30571 | C | -0.61867 | -4.76145 | -1.05923 | C | 1.31556  | -1.27930 | -0.76612 |
| C | -4.32028 | 3.83903  | -2.91165 | C | 0.60160  | -4.54769 | -1.73346 | C | -0.07555 | -1.25802 | -0.83184 |
| C | -5.52104 | 4.31841  | -2.31630 | C | 0.60496  | -3.78102 | -2.93987 | C | -0.77095 | -0.05196 | -0.93934 |
| C | -5.52232 | 4.82849  | -1.04638 | C | -0.61179 | -3.26651 | -3.43144 | C | -0.03808 | 1.13630  | -0.93887 |
| C | -1.85908 | 3.79944  | -2.87978 | C | -0.60954 | -2.04066 | -4.16252 | H | 3.12155  | -0.10549 | -0.77330 |
| C | -1.85328 | 2.73744  | -3.79799 | C | 0.60904  | -1.36967 | -4.37837 | H | 1.84056  | -2.22576 | -0.67794 |
| C | -3.09293 | 2.11516  | -4.16225 | C | 0.60813  | 0.04418  | -4.55917 | H | -0.63766 | -2.18839 | -0.79768 |
| C | -4.31318 | 2.75840  | -3.87641 | C | -0.61122 | 0.74685  | -4.52630 | C | -2.27638 | -0.03267 | -1.02495 |
| C | -3.08735 | 0.74107  | -4.56099 | C | -0.61507 | 2.12220  | -4.14735 | H | -0.57093 | 2.08277  | -0.98890 |
| C | -4.30216 | 0.03804  | -4.68338 | C | 0.60046  | 2.75473  | -3.82051 | H | -2.62904 | 0.85627  | -1.55930 |
| C | -5.50096 | 0.80446  | -4.69979 | C | 0.59554  | 3.84243  | -2.89496 | H | -2.65315 | -0.91840 | -1.54877 |
| C | -5.50676 | 2.11622  | -4.30951 | C | -0.62559 | 4.52026  | -2.31938 | H | -2.72858 | -0.02126 | -0.02704 |
| C | -1.84308 | 0.03062  | -4.57506 | C | 1.83290  | 3.73626  | 2.99709  | H | 1.90798  | 2.05616  | -0.87953 |
| C | -1.84217 | -1.36171 | -4.39275 | C | 3.07712  | 3.25304  | 3.51912  | H | -6.45362 | -3.77666 | -3.35548 |
| C | -3.08629 | -2.04423 | -4.19255 | C | 3.08081  | 2.04762  | 4.29053  | H | -6.44607 | -1.74005 | -4.64599 |
| C | -4.30170 | -1.39777 | -4.49131 | C | 1.83951  | 1.36934  | 4.51941  | H | -6.44676 | 0.32396  | -4.92425 |
| C | -3.09018 | -3.25914 | -3.43640 | C | 1.84092  | -0.02159 | 4.70950  | H | -6.45676 | 2.63369  | -2.36066 |
| C | -4.30932 | -3.79674 | -2.97862 | C | 3.08359  | -0.73431 | 4.67060  | H | -6.46992 | 4.18025  | -2.82232 |
| C | -5.50426 | -3.29840 | -3.56946 | C | 3.08246  | -2.10336 | 4.25463  | H | -6.47164 | 5.07711  | -0.58504 |
| C | -5.49986 | -2.14110 | -4.30047 | C | 1.83900  | -2.71310 | 3.88587  | H | -6.46365 | 4.91204  | 1.50665  |
| C | -1.84929 | -3.75751 | -2.91834 | C | 1.83677  | -3.75838 | 2.94911  | H | -6.45766 | 3.65496  | 3.56443  |
| C | -1.85329 | -4.50409 | -1.72869 | C | 3.07845  | -4.19593 | 2.38404  | H | -6.45414 | 1.89390  | 4.69429  |
| C | -3.09833 | -4.73196 | -1.05536 | C | 3.07717  | -4.75266 | 1.06590  | H | -6.45283 | -0.49280 | 5.02391  |
| C | -4.31366 | -4.55526 | -1.74430 | C | 1.83491  | -4.85302 | 0.35669  | H | -6.45217 | -2.49432 | 4.41421  |
| C | -3.09869 | -4.84340 | 0.37115  | C | 1.83612  | -4.75696 | -1.04554 | H | -6.45612 | -4.27988 | 2.79534  |
| C | -4.31441 | -4.78040 | 1.07986  | C | 3.08115  | -4.54299 | -1.72478 | H | -6.46226 | -5.05975 | 0.84418  |
| C | -5.51314 | -4.95198 | 0.33121  | C | 3.08296  | -3.77214 | -2.93148 | H | -6.46133 | -4.86356 | -1.55816 |
| C | -5.51292 | -4.84172 | -1.03295 | C | 1.84055  | -3.24918 | -3.41741 | H | 6.44206  | 2.51306  | -4.27781 |
| C | -1.85357 | -4.71354 | 1.06944  | C | 1.84204  | -2.04032 | -4.13195 | H | 6.43854  | 4.33198  | -2.69548 |
| C | -1.85175 | -4.17246 | 2.36438  | C | 3.08291  | -1.37019 | -4.38219 | H | 6.43204  | 5.13693  | -0.75194 |
| C | -3.09334 | -3.77808 | 2.96283  | C | 3.08208  | 0.04824  | -4.56833 | H | 6.43093  | 4.90469  | 1.64786  |
| C | -4.31154 | -4.23345 | 2.42126  | C | 1.84006  | 0.75804  | -4.49711 | H | 6.43907  | 3.77720  | 3.41461  |
| C | -3.09144 | -2.71745 | 3.92303  | C | 1.83638  | 2.11289  | -4.13061 | H | 6.44462  | 1.74634  | 4.71280  |
| C | -4.30729 | -2.13117 | 4.32702  | C | 3.07807  | 2.75359  | -3.81521 | H | 6.44759  | -0.32337 | 4.99150  |
| C | -5.50475 | -2.83089 | 4.00813  | C | 3.07485  | 3.84088  | -2.88497 | H | 6.44560  | -2.62969 | 4.29610  |
| C | -5.50702 | -3.84509 | 3.08857  | C | 1.82960  | 4.24786  | -2.30148 | H | 6.43998  | -4.20722 | 2.91947  |
| C | -1.84807 | -2.08482 | 4.25092  | C | 4.29175  | 3.79436  | 3.05399  | H | 6.43931  | -5.13402 | 0.69404  |
| C | -1.84768 | -0.74352 | 4.66430  | C | 5.49171  | 3.29947  | 3.63826  | H | 6.44461  | -4.95066 | -1.39850 |
| C | -3.09076 | -0.03489 | 4.74885  | C | 5.49490  | 2.14539  | 4.37449  | H | 6.44728  | -3.66270 | -3.43787 |
| C | -4.30707 | -0.74595 | 4.75208  | C | 4.29883  | 1.40320  | 4.58307  | H | 6.44595  | -1.88113 | -4.52764 |
| C | -3.09185 | 1.38308  | 4.55455  | C | 4.30046  | -0.03258 | 4.77953  | H | 6.44464  | 0.50649  | -4.84829 |
| C | -4.30926 | 2.06661  | 4.36625  | C | 5.49807  | -0.80150 | 4.77772  |   |          |          |          |
| C | -5.50543 | 1.36882  | 4.69344  | C | 5.49686  | -2.11186 | 4.38214  |   |          |          |          |
| C | -5.50441 | 0.01250  | 4.87997  | C | 4.29804  | -2.75001 | 3.95664  |   |          |          |          |

Toluene-graphene, gas

C 5.13382 0.74995 -0.19219  
 C 5.83591 -0.48357 -0.15326  
 C 7.27202 -0.48125 -0.10013  
 C 7.96141 0.75818 -0.09224  
 C 7.28863 1.95619 -0.13468  
 C 5.84951 1.96430 -0.18479  
 C 5.13051 -1.70561 -0.16696  
 C 5.84430 -2.93052 -0.12865  
 C 7.27492 -2.91672 -0.07133  
 C 7.95512 -1.69240 -0.05950  
 C 5.15267 -4.17769 -0.14494  
 C 5.89310 -5.35133 -0.09879  
 C 7.29799 -5.33511 -0.04126  
 C 7.98056 -4.14671 -0.02874  
 C 3.69352 -1.69871 -0.22112  
 C 2.98287 -2.93483 -0.24054  
 C 3.68917 -4.16819 -0.20957  
 C 3.70250 0.75899 -0.24191  
 C 2.99032 -0.47883 -0.25511  
 C 1.55597 -2.92636 -0.29590  
 C 0.84428 -4.15306 -0.31266  
 C 1.57136 -5.34422 -0.29785  
 C 2.95245 -5.35065 -0.24777  
 C 0.84568 -1.68681 -0.33444  
 C 1.55817 -0.47054 -0.31182  
 C -0.58745 -1.67955 -0.39709  
 C -1.31009 -2.91172 -0.40078  
 C -0.61266 -4.14504 -0.34658  
 C 3.00483 1.98212 -0.27762  
 C 1.57195 1.99025 -0.32317  
 C 0.85776 0.77295 -0.33880  
 C -0.57316 0.77955 -0.38479  
 C -1.28667 -0.45624 -0.40525  
 C -2.71835 -0.44964 -0.43048  
 C -3.43433 -1.66188 -0.43845  
 C -2.73702 -2.90492 -0.43135  
 C -3.45699 -4.13031 -0.41927  
 C -2.73445 -5.31978 -0.34357  
 C -1.35290 -5.32777 -0.30724  
 C -4.87206 -1.65450 -0.42184  
 C -5.60013 -2.87161 -0.44073  
 C -4.92105 -4.12538 -0.46398  
 C -5.56498 -0.42584 -0.38306  
 C -4.84883 0.79992 -0.36376  
 C -3.41649 0.79419 -0.39118  
 C -2.70568 2.00999 -0.36737  
 C -1.27285 2.00432 -0.37595  
 C -0.55776 3.24028 -0.35933  
 C 0.87008 3.23384 -0.34528  
 C 7.03148 -2.84348 -0.44156  
 C -7.75014 -4.06609 -0.48663  
 C -7.07924 -5.26022 -0.53412  
 C -5.67337 -5.29067 -0.52371  
 C -7.69896 -1.61287 -0.39934  
 C -7.00183 -0.40930 -0.36467  
 C -7.67780 0.83644 -0.31484  
 C -6.99139 2.02720 -0.28666  
 C -5.55168 2.02091 -0.31358  
 C -4.84002 3.24822 -0.29124  
 C -3.41578 3.24953 -0.32032  
 C -2.71753 4.48315 -0.30500  
 C -1.26076 4.47419 -0.33802  
 C -5.55443 4.47518 -0.24069  
 C -6.99439 4.45759 -0.21010  
 C -7.67940 3.29434 -0.23249  
 C -3.45510 5.67427 -0.25241  
 C -4.83803 5.67180 -0.22077  
 C 1.58636 4.46052 -0.33456  
 C 0.85858 5.65280 -0.34030  
 C -0.52107 5.65933 -0.33900  
 C 3.04326 4.45511 -0.30843  
 C 3.72815 3.21471 -0.27128  
 C 5.15180 3.19887 -0.22712  
 C 5.87959 4.41910 -0.22469  
 C 5.17673 5.62285 -0.27045

C 3.79398 5.63911 -0.31108  
 C 7.99047 3.21688 -0.13107  
 C 7.31871 4.38719 -0.17527  
 H -7.51610 5.40956 -0.16863  
 H 7.85099 5.33425 -0.17369  
 H -8.78595 -1.59947 -0.39388  
 H -8.76482 0.84008 -0.29818  
 H -8.76525 3.28505 -0.21027  
 H -8.83560 -4.03389 -0.48859  
 H -7.62892 -6.19468 -0.57925  
 H -5.18616 -6.25681 -0.57107  
 H -3.25002 -6.27103 -0.29696  
 H -0.85499 -6.28612 -0.23460  
 H 1.06252 -6.29886 -0.33358  
 H 3.45566 -6.30949 -0.23994  
 H 5.39748 -6.31418 -0.10496  
 H 7.83753 -6.27596 -0.00663  
 H 9.06539 -4.12507 0.01473  
 H 9.04138 -1.69029 -0.01800  
 H 9.04778 0.75076 -0.05362  
 H 9.07575 3.19684 -0.09297  
 H -5.37976 6.61247 -0.17933  
 H -2.94735 6.63013 -0.23156  
 H -1.02298 6.61848 -0.33669  
 H 1.36973 6.60699 -0.33549  
 H 3.29738 6.60043 -0.34703  
 H 5.72902 6.55825 -0.27265  
 C -1.85365 -1.96702 2.79947  
 C -0.50847 -1.60114 2.83111  
 C -0.15142 -0.25736 2.86359  
 C -1.12745 0.74463 2.87054  
 C -2.47062 0.36618 2.83996  
 C -2.83354 -0.97906 2.80688  
 H 0.26409 -2.36523 2.80187  
 H 0.89935 0.02448 2.86662  
 C -0.73318 2.19859 2.91510  
 H -3.24025 1.13506 2.82229  
 H -3.88408 -1.25362 2.76107  
 H -1.51661 2.83433 2.49145  
 H -0.55738 2.52496 3.94612  
 H 0.18968 2.37288 2.35137  
 H -2.13352 -3.01550 2.74889

Toluene-convex surface of  
SWCNT, gas

C -3.67048 -5.81621 -1.82107  
 C -3.33833 -4.60487 -2.49089  
 C -3.70146 -3.39934 -1.85895  
 C -4.06920 -3.40045 -0.47541  
 C -4.07529 -4.60821 0.25001  
 C -4.02695 -5.81765 -0.49959  
 C -3.43878 -2.14635 -2.50378  
 C -3.87220 -0.92740 -1.90031  
 C -4.22577 -0.92823 -0.51870  
 C -4.16063 -2.14872 0.21659  
 C -3.63089 0.30056 -2.54854  
 C -4.02899 1.52067 -1.92642  
 C -4.37614 1.51794 -0.56752  
 C -4.33522 0.29708 0.16531  
 C -3.80743 2.77206 -2.58971  
 C -4.27247 3.96800 -2.00791  
 C -4.64639 3.96287 -0.60676  
 C -4.52083 2.76510 0.12279  
 C -4.26919 2.80768 1.53008  
 C -4.13364 4.04866 2.18352  
 C -4.58556 5.20321 1.48425  
 C -4.83442 5.16106 0.13800  
 C -3.88252 1.60102 2.19927  
 C -3.06103 1.67798 3.33477  
 C -2.62551 2.96311 3.79631  
 C -3.28047 4.12912 3.35238  
 C -1.36476 3.06216 4.46639  
 C -0.78168 4.32657 4.68168  
 C -1.61927 5.46584 4.52014

C -2.82465 5.37093 3.87798  
 C -0.58507 1.87335 4.65148  
 C 0.81433 1.97237 4.70072  
 C 1.43075 3.25965 4.56686  
 C 0.66252 4.42838 4.73488  
 C 2.73810 3.34158 3.99034  
 C 3.25423 4.59069 3.59331  
 C 2.59309 5.75284 4.08093  
 C 1.34261 5.67473 4.63182  
 C 3.38401 2.13363 3.56823  
 C 4.29750 2.18025 2.50332  
 C 4.56280 3.43427 1.86180  
 C 4.19670 4.63872 2.49398  
 C 4.93403 3.43749 0.47958  
 C 4.93273 4.64491 -0.24614  
 C 4.87975 5.85421 0.50272  
 C 4.52489 5.85112 1.82451  
 C 5.02789 2.18628 -0.21317  
 C 4.77240 2.14453 -1.59306  
 C 4.42338 3.35463 -2.27750  
 C 4.66912 4.60191 -1.67028  
 C 3.57997 3.27612 -3.43099  
 C 2.99776 4.44610 -3.95723  
 C 3.53166 5.69160 -3.52160  
 C 4.33829 5.76679 -2.41854  
 C 3.11509 1.98991 -3.86032  
 C 1.87891 1.89235 -4.51883  
 C 1.11077 3.08078 -4.74721  
 C 1.72215 4.34543 -4.63707  
 C -0.31539 2.97964 -4.80321  
 C -1.10510 4.14519 -4.74648  
 C -0.44822 5.38774 -4.97094  
 C 0.91618 5.48453 -4.91798  
 C -0.92417 1.69339 -4.62828  
 C -2.20790 1.61317 -4.06551  
 C -2.87939 2.81927 -3.67758  
 C -2.42915 4.06282 -4.16334  
 C -4.05176 5.17240 -2.73254  
 C -3.16247 5.21837 -3.77281  
 C -2.70541 0.34693 -3.63427  
 C -2.05303 -0.83666 -4.03335  
 C -0.74792 -0.75480 -4.60520  
 C -0.14046 0.50787 -4.75730  
 C 1.28216 0.60887 -4.70127  
 C 2.04773 -0.55594 -4.49632  
 C 3.30471 -0.45679 -3.82705  
 C 3.75160 0.80448 -3.38533  
 C 4.59280 0.88280 -2.23484  
 C 4.95768 -0.30243 -1.56607  
 C 5.21778 -0.25993 -0.16321  
 C 5.10396 0.96581 0.52219  
 C 4.73352 0.96254 1.90068  
 C 4.48890 -0.26604 2.54574  
 C 3.55999 -0.31352 3.62829  
 C 2.90801 0.86968 4.02869  
 C 1.60436 0.78785 4.60414  
 C 0.99716 -0.47466 4.75744  
 C -0.42559 -0.57547 4.70744  
 C -1.19151 0.58970 4.50532  
 C -2.44976 0.49098 3.83858  
 C -2.89644 -0.76986 3.39488  
 C -3.73389 -0.84719 2.24160  
 C -4.08696 0.33850 1.56829  
 C -2.52837 -2.10077 -3.57120  
 C -1.88137 -3.30905 -3.99040  
 C -0.57328 -3.22686 -4.56531  
 C 0.04278 -1.93925 -4.69844  
 C 1.44195 -1.83963 -4.64418  
 C 2.22184 -3.02779 -4.45812  
 C 3.48215 -2.92822 -3.78724  
 C 3.91819 -1.64340 -3.32517  
 C 4.74586 -1.56617 -2.19383  
 C 5.13587 -2.77360 -1.52699  
 C 5.39683 -2.73084 -0.12045  
 C 5.25866 -1.48282 0.57080



|   |          |          |          |
|---|----------|----------|----------|
| C | 4.89409  | -1.48607 | 1.92656  |
| C | 4.66727  | -2.73716 | 2.58817  |
| C | 3.73554  | -2.78486 | 3.67323  |
| C | 3.06311  | -1.57956 | 4.06013  |
| C | 1.78050  | -1.66011 | 4.62556  |
| C | 1.17228  | -2.94628 | 4.80167  |
| C | -0.25409 | -3.04747 | 4.74982  |
| C | -1.02294 | -1.85885 | 4.52524  |
| C | -2.26051 | -1.95590 | 3.86910  |
| C | -2.72545 | -3.24165 | 3.43783  |
| C | -3.56836 | -3.31904 | 2.28346  |
| C | -3.91296 | -2.10791 | 1.59812  |
| C | -2.39643 | -4.55802 | -3.59078 |
| C | -1.73380 | -5.72051 | -4.07567 |
| C | -0.48312 | -5.64216 | -4.62602 |
| C | 0.19600  | -4.39526 | -4.73052 |
| C | 1.63995  | -4.29240 | -4.67556 |
| C | 2.47861  | -5.43108 | -4.51580 |
| C | 3.68376  | -5.33576 | -3.87358 |
| C | 4.13802  | -4.09424 | -3.34575 |
| C | 4.99263  | -4.01454 | -2.17842 |
| C | 5.43845  | -5.17162 | -1.47933 |
| C | 5.68850  | -5.13066 | -0.13401 |
| C | 5.51059  | -3.93018 | 0.60957  |
| C | 5.13361  | -3.93369 | 2.00858  |
| C | 4.91307  | -5.13782 | 2.73434  |
| C | 4.02153  | -5.18360 | 3.77211  |
| C | 3.28560  | -4.02835 | 4.15926  |
| C | 1.96207  | -4.11165 | 4.74264  |
| C | 1.30581  | -5.35464 | 4.96707  |
| C | -0.05864 | -5.45148 | 4.91700  |
| C | -0.86558 | -4.31210 | 4.63958  |
| C | -2.14255 | -4.41220 | 3.96215  |
| C | -2.67673 | -5.65736 | 3.52554  |
| C | -3.48354 | -5.73156 | 2.42252  |
| C | -3.81371 | -4.56594 | 1.67489  |
| H | 3.03202  | 6.73174  | 3.92339  |
| H | 0.82959  | 6.59390  | 4.89175  |
| H | -1.26000 | 6.44702  | 4.80953  |
| H | -3.38057 | 6.27987  | 3.67634  |
| H | -4.63581 | 6.15944  | 1.99334  |
| H | -5.07450 | 6.08523  | -0.37610 |
| H | -4.50601 | 6.09750  | -2.39520 |
| H | -2.94291 | 6.17811  | -4.22711 |
| H | -1.03035 | 6.29630  | -5.07848 |
| H | 1.37143  | 6.46617  | -4.98773 |
| H | 3.21595  | 6.61260  | -3.99896 |
| H | 4.63662  | 6.74449  | -2.05684 |
| H | 5.01695  | 6.80677  | 0.00329  |
| H | 4.39232  | 6.80147  | 2.32942  |
| H | -2.36064 | -6.57885 | 4.00172  |
| H | -3.78115 | -6.70907 | 2.05965  |
| H | -4.16892 | -6.76973 | -0.00046 |
| H | -3.54140 | -6.76707 | -2.32597 |
| H | -2.17149 | -6.69958 | -3.91564 |
| H | 0.03114  | -6.56134 | -4.88339 |
| H | 2.12096  | -6.41198 | -4.80811 |
| H | 4.24170  | -6.24410 | -3.67512 |
| H | 5.48153  | -6.12822 | -1.98818 |
| H | 5.92142  | -6.05608 | 0.38084  |
| H | 5.37171  | -6.06198 | 2.40064  |
| H | 3.80354  | -6.14259 | 4.22873  |
| H | 1.88824  | -6.26329 | 5.07218  |
| H | -0.51359 | -6.43329 | 4.98642  |
| C | -7.60107 | 1.30742  | -0.54929 |
| C | -7.53696 | 0.06913  | -1.17764 |
| C | -7.42598 | -1.10976 | -0.43286 |
| C | -7.37690 | -1.01547 | 0.95813  |
| C | -7.43389 | 0.22483  | 1.59261  |
| C | -7.54661 | 1.39051  | 0.84139  |
| H | -7.55641 | 0.01115  | -2.26350 |
| C | -7.32995 | -2.44088 | -1.13222 |
| H | -7.27495 | -1.92206 | 1.54978  |
| H | -7.37539 | 0.27894  | 2.67566  |
| H | -7.57546 | 2.35878  | 1.33225  |

|   |          |          |          |
|---|----------|----------|----------|
| H | -7.10601 | -3.24612 | -0.42809 |
| H | -8.26562 | -2.68584 | -1.64515 |
| H | -6.53592 | -2.42501 | -1.88756 |
| H | -7.66493 | 2.21400  | -1.14457 |

# Benzene-concave surface of SWCNT, gas

|   |          |          |          |
|---|----------|----------|----------|
| C | -0.08725 | 1.14929  | -0.91539 |
| C | 1.30658  | 1.13658  | -0.88926 |
| C | 1.99165  | -0.07483 | -0.84276 |
| C | 1.28124  | -1.27119 | -0.79022 |
| C | -0.11239 | -1.25839 | -0.81924 |
| C | -0.79731 | -0.04860 | -0.89839 |
| H | -1.88344 | -0.03857 | -0.93070 |
| C | -0.59223 | -3.22466 | -3.48072 |
| C | -1.83446 | -3.72482 | -2.98862 |
| C | -3.07011 | -3.21890 | -3.51126 |
| C | -3.05956 | -1.99306 | -4.24872 |
| C | -1.81384 | -1.30810 | -4.42873 |
| C | -0.58330 | -1.98974 | -4.19628 |
| C | -4.27200 | -1.34429 | -4.55474 |
| C | -4.27118 | 0.09382  | -4.73120 |
| C | -3.05803 | 0.79581  | -4.58678 |
| C | -1.81336 | 0.08594  | -4.59578 |
| C | -0.58241 | 0.80211  | -4.52855 |
| C | -0.59088 | 2.17331  | -4.13506 |
| C | -1.83261 | 2.78498  | -3.79248 |
| C | -3.06815 | 2.16544  | -4.17416 |
| C | -4.29130 | 2.80777  | -3.89898 |
| C | -4.30902 | 3.88073  | -2.92552 |
| C | -3.10144 | 4.24949  | -2.30167 |
| C | -1.84860 | 3.83871  | -2.86516 |
| C | -0.62142 | 4.28207  | -2.28536 |
| C | -0.63860 | 4.78949  | -0.94906 |
| C | -1.88099 | 4.84561  | -0.24734 |
| C | -3.11798 | 4.76538  | -0.96792 |
| C | 0.57265  | 4.87789  | -0.23295 |
| C | 0.55803  | 4.70939  | 1.18527  |
| C | -0.66646 | 4.46785  | 1.83890  |
| C | -1.89488 | 4.68645  | 1.14789  |
| C | 1.81659  | 4.77948  | -0.92729 |
| C | 3.05070  | 4.88573  | -0.20448 |
| C | 3.03499  | 4.72268  | 1.21779  |
| C | 1.78593  | 4.45646  | 1.86669  |
| C | 4.27653  | 4.85089  | -0.89744 |
| C | 5.46448  | 5.01303  | -0.12923 |
| C | 5.44826  | 4.86407  | 1.23088  |
| C | 4.24388  | 4.54170  | 1.91786  |
| C | 1.77620  | 3.70077  | 3.05028  |
| C | 3.01452  | 3.21148  | 3.58070  |
| C | 4.23414  | 3.75928  | 3.13689  |
| C | 1.83337  | 4.27942  | -2.24021 |
| C | 3.08508  | 3.87854  | -2.81431 |
| C | 4.29471  | 4.32566  | -2.24661 |
| C | 0.53786  | 3.20145  | 3.55214  |
| C | -0.67692 | 3.70184  | 3.04358  |
| C | 0.60594  | 3.88004  | -2.85154 |
| C | -1.91516 | 3.18152  | 3.52469  |
| C | -3.15388 | 3.70222  | 3.02669  |
| C | -3.14367 | 4.46720  | 1.81718  |
| C | -4.35471 | 4.75198  | 1.15712  |
| C | -4.34167 | 4.90256  | -0.28396 |
| C | -4.37476 | 3.23821  | 3.55512  |
| C | -5.56812 | 3.82565  | 3.04828  |
| C | -5.55857 | 4.55592  | 1.89050  |
| C | -5.51637 | 4.35460  | -2.33892 |
| C | -5.53221 | 4.84914  | -1.06293 |
| C | 0.62110  | 2.80234  | -3.78849 |
| C | -5.46952 | 0.86078  | -4.75345 |
| C | -5.47966 | 2.16919  | -4.35119 |
| C | 0.63747  | 0.10024  | -4.55718 |
| C | 0.63707  | -1.31576 | -4.39238 |
| C | -4.29339 | -3.76580 | -3.07661 |
| C | -5.48223 | -3.25920 | -3.67261 |
| C | -5.47123 | -2.09130 | -4.38689 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.85032 | -4.49058 | -1.81122 |
| C | -3.10241 | -4.73025 | -1.15514 |
| C | -4.31014 | -4.54423 | -1.85480 |
| C | 0.61989  | -3.74539 | -2.98431 |
| C | 0.60457  | -4.52908 | -1.78888 |
| C | -0.62276 | -4.75498 | -1.13154 |
| C | -0.63957 | -4.87171 | 0.29317  |
| C | -1.88170 | -4.73547 | 0.98369  |
| C | -3.11873 | -4.85934 | 0.26994  |
| C | -4.34231 | -4.80520 | 0.96562  |
| C | -5.53248 | -4.96921 | 0.20156  |
| C | -5.51697 | -4.84167 | -1.16095 |
| C | -1.89516 | -4.20765 | 2.28416  |
| C | -3.14389 | -3.82045 | 2.87246  |
| C | -4.35530 | -4.27175 | 2.31250  |
| C | 0.57172  | -4.76056 | 1.00489  |
| C | 0.55777  | -4.21810 | 2.32494  |
| C | -0.66658 | -3.81318 | 2.89177  |
| C | -0.67683 | -2.76289 | 3.85762  |
| C | -1.91519 | -2.13844 | 4.19128  |
| C | -3.15405 | -2.76874 | 3.84254  |
| C | -4.37497 | -2.18734 | 4.23803  |
| C | -5.56799 | -2.88500 | 3.89857  |
| C | -5.55873 | -3.89050 | 2.96956  |
| C | -1.92079 | -0.80172 | 4.61909  |
| C | -3.16523 | -0.09473 | 4.69680  |
| C | -4.38095 | -0.80664 | 4.67754  |
| C | 0.53808  | -2.15097 | 4.22314  |
| C | 0.53290  | -0.79207 | 4.65695  |
| C | -0.68756 | -0.09052 | 4.71197  |
| C | -0.68752 | 1.32547  | 4.53519  |
| C | -1.92064 | 1.99161  | 4.27020  |
| C | -3.16497 | 1.32550  | 4.51927  |
| C | -4.38052 | 2.01063  | 4.32499  |
| C | -5.57999 | 1.30811  | 4.62898  |
| C | -5.58025 | -0.05031 | 4.79952  |
| C | 0.53280  | 1.99211  | 4.30956  |
| C | 3.00993  | 1.99663  | 4.33712  |
| C | 1.76643  | 1.31497  | 4.54290  |
| C | 1.76653  | -0.07810 | 4.71676  |
| C | 3.01012  | -0.78961 | 4.68459  |
| C | 3.01507  | -2.15378 | 4.25311  |
| C | 1.77645  | -2.76017 | 3.86294  |
| C | 1.78601  | -3.79537 | 2.91509  |
| C | 3.03458  | -4.22527 | 2.35938  |
| C | 3.04902  | -4.76601 | 1.03475  |
| C | 1.81494  | -4.85943 | 0.31055  |
| C | 1.83178  | -4.74523 | -1.09017 |
| C | 3.08384  | -4.52053 | -1.75271 |
| C | 3.09764  | -3.73460 | -2.94967 |
| C | 1.85991  | -3.20670 | -3.44245 |
| C | 1.86794  | -1.98908 | -4.14222 |
| C | 3.11099  | -1.31535 | -4.37190 |
| C | 3.11149  | 0.10533  | -4.54196 |
| C | 1.86850  | 0.81407  | -4.47585 |
| C | 1.86048  | 2.16463  | -4.09328 |
| C | 3.09848  | 2.80193  | -3.75692 |
| C | 5.42739  | 3.25798  | 3.72928  |
| C | 5.42271  | 2.09495  | 4.45140  |
| C | 4.22484  | 1.34951  | 4.63655  |
| C | 4.22509  | -0.08845 | 4.81630  |
| C | 5.42324  | -0.85656 | 4.81990  |
| C | 5.42781  | -2.16228 | 4.40913  |
| C | 4.23458  | -2.79625 | 3.96223  |
| C | 4.24409  | -3.86734 | 2.98669  |
| C | 5.44776  | -4.36275 | 2.41040  |
| C | 5.46267  | -4.87498 | 1.14150  |
| C | 4.27428  | -4.92797 | 0.35890  |
| C | 4.29263  | -4.79469 | -1.08320 |
| C | 5.50059  | -4.58977 | -1.80812 |
| C | 5.51355  | -3.84374 | -2.95502 |
| C | 4.32031  | -3.25005 | -3.45564 |
| C | 4.32727  | -2.00394 | -4.19346 |
| C | 5.52681  | -1.29845 | -4.48826 |
| C | 5.52703  | 0.06061  | -4.65354 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 4.32774  | 0.81667  | -4.53475 |
| C | 4.32087  | 2.20621  | -4.12697 |
| C | 5.51387  | 2.90970  | -3.79912 |
| C | 5.50203  | 3.93258  | -2.89013 |
| H | 3.07777  | -0.08614 | -0.83146 |
| H | 1.81705  | -2.21289 | -0.71840 |
| H | -0.66837 | -2.19011 | -0.77282 |
| H | -0.62377 | 2.09313  | -0.94481 |
| H | 1.86163  | 2.07042  | -0.89794 |
| H | -6.43351 | -3.74115 | -3.47607 |
| H | -6.41416 | -1.68651 | -4.73710 |
| H | -6.41277 | 0.38262  | -4.99325 |
| H | -6.43050 | 2.68604  | -4.28400 |
| H | -6.45937 | 4.22319  | -2.85761 |
| H | -6.48680 | 5.09273  | -0.60979 |
| H | -6.50321 | 4.89514  | 1.48018  |
| H | -6.52030 | 3.60908  | 3.51972  |
| H | -6.52907 | 1.83251  | 4.62452  |
| H | -6.53005 | -0.55760 | 4.92627  |
| H | -6.52039 | -2.55312 | 4.29679  |
| H | -6.50404 | -4.32298 | 2.66099  |
| H | -6.48712 | -5.08428 | 0.70257  |
| H | -6.45929 | -4.85726 | -1.69723 |
| H | 6.46746  | 2.56760  | -4.18568 |
| H | 6.44632  | 4.36695  | -2.58125 |
| H | 6.41814  | 5.14659  | -0.62751 |
| H | 6.38913  | 4.88532  | 1.76949  |
| H | 6.37705  | 3.73893  | 3.52292  |
| H | 6.36866  | 1.69249  | 4.79618  |
| H | 6.36968  | -0.38028 | 5.05077  |
| H | 6.37788  | -2.67853 | 4.32843  |
| H | 6.38981  | -4.23988 | 2.93293  |
| H | 6.41561  | -5.13909 | 0.69639  |
| H | 6.44406  | -4.92849 | -1.39476 |
| H | 6.46718  | -3.61585 | -3.41802 |
| H | 6.47580  | -1.82302 | -4.48815 |
| H | 6.47666  | 0.56796  | -4.78107 |

# Benzene-graphene, gas

|   |          |          |          |
|---|----------|----------|----------|
| C | -2.71582 | -0.91723 | 2.87802  |
| C | -1.74100 | -1.91107 | 2.86197  |
| C | -0.39061 | -1.56323 | 2.87591  |
| C | -0.01709 | -0.22237 | 2.90042  |
| C | -0.99408 | 0.77246  | 2.91470  |
| C | -2.34268 | 0.42614  | 2.90370  |
| H | -0.70156 | 1.81892  | 2.91505  |
| C | -0.61020 | -1.64289 | -0.35325 |
| C | 0.82333  | -1.65190 | -0.30682 |
| C | 1.53314  | -2.89220 | -0.29008 |
| C | 0.82019  | -4.11808 | -0.30531 |
| C | -0.63688 | -4.10834 | -0.30548 |
| C | -1.33399 | -2.87438 | -0.34805 |
| C | 1.53665  | -0.43645 | -0.27755 |
| C | 2.96925  | -0.44660 | -0.22974 |
| C | 3.67214  | -1.66717 | -0.22641 |
| C | 2.96058  | -2.90250 | -0.25778 |
| C | 3.68186  | 0.79023  | -0.19395 |
| C | 5.11368  | 0.77967  | -0.15513 |
| C | 5.81561  | -0.45451 | -0.15385 |
| C | 5.10955  | -1.67576 | -0.18829 |
| C | 7.25218  | -0.45388 | -0.11620 |
| C | 7.94204  | 0.78481  | -0.08222 |
| C | 7.26941  | 1.98364  | -0.08431 |
| C | 5.82996  | 1.99334  | -0.12113 |
| C | 2.98426  | 2.01388  | -0.19361 |
| C | 3.70817  | 3.24562  | -0.15721 |
| C | 5.13206  | 3.22847  | -0.12281 |
| C | 5.82293  | -2.90150 | -0.18555 |
| C | 7.25417  | -2.88942 | -0.14742 |
| C | 7.93505  | -1.66584 | -0.11406 |
| C | 5.86022  | 4.44810  | -0.09070 |
| C | 7.29985  | 4.41488  | -0.05431 |
| C | 7.97165  | 3.24377  | -0.05069 |
| C | 3.66618  | -4.13662 | -0.25852 |
| C | 5.13051  | -4.14786 | -0.21947 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.87078  | -5.32249 | -0.21177 |
| C | 7.27633  | -5.30794 | -0.17494 |
| C | 7.95960  | -4.12029 | -0.14385 |
| C | 1.54604  | -5.30999 | -0.32368 |
| C | 2.92788  | -5.31806 | -0.30149 |
| C | 1.55134  | 2.02343  | -0.23563 |
| C | 0.83658  | 0.80734  | -0.27939 |
| C | -1.30848 | -0.41893 | -0.34841 |
| C | -0.59400 | 0.81584  | -0.32453 |
| C | -2.74079 | -0.41127 | -0.36912 |
| C | -3.45775 | -1.62295 | -0.36918 |
| C | -2.76129 | -2.86656 | -0.35960 |
| C | -3.48208 | -4.09161 | -0.33319 |
| C | -2.75929 | -5.28112 | -0.25979 |
| C | -1.37728 | -5.29017 | -0.24536 |
| C | 3.02361  | 4.48660  | -0.15590 |
| C | 1.56678  | 4.49290  | -0.18291 |
| C | 0.84996  | 3.26692  | -0.22417 |
| C | -0.57791 | 3.27527  | -0.25337 |
| C | -1.29369 | 2.04065  | -0.29848 |
| C | -2.72647 | 2.04826  | -0.30790 |
| C | -3.43836 | 0.83304  | -0.33556 |
| C | -4.87075 | 0.84036  | -0.32557 |
| C | -5.58796 | -0.38513 | -0.33796 |
| C | -4.89569 | -1.61462 | -0.35679 |
| C | -5.62438 | -2.83151 | -0.36178 |
| C | -4.94638 | -4.08606 | -0.36628 |
| C | -7.02490 | -0.36728 | -0.33254 |
| C | -7.72256 | -1.57086 | -0.35077 |
| C | -7.05581 | -2.80244 | -0.36702 |
| C | -7.77538 | -4.02509 | -0.39045 |
| C | -7.10552 | -5.22057 | -0.41255 |
| C | -5.69971 | -5.25181 | -0.40189 |
| C | -7.70029 | 0.87954  | -0.31103 |
| C | -7.01313 | 2.07004  | -0.29280 |
| C | -5.57317 | 2.06225  | -0.29803 |
| C | -4.86059 | 3.28900  | -0.27565 |
| C | -3.43614 | 3.28858  | -0.27496 |
| C | -2.73712 | 4.52118  | -0.24438 |
| C | -1.28025 | 4.51010  | -0.22965 |
| C | -0.53968 | 5.69364  | -0.18660 |
| C | 0.83989  | 5.68539  | -0.16536 |
| C | -5.57448 | 4.51707  | -0.25070 |
| C | -7.01486 | 4.50123  | -0.24889 |
| C | -7.70067 | 3.33847  | -0.26842 |
| C | -4.85737 | 5.71314  | -0.22778 |
| C | -3.47412 | 5.71367  | -0.22423 |
| C | 5.15746  | 5.65273  | -0.09576 |
| C | 3.77457  | 5.67018  | -0.12760 |
| H | -7.53615 | 5.45419  | -0.23015 |
| H | 7.83213  | 5.36156  | -0.02914 |
| H | -8.80954 | -1.55670 | -0.35216 |
| H | -8.78745 | 0.88423  | -0.30780 |
| H | -8.78675 | 3.33032  | -0.26587 |
| H | -8.86080 | -3.99194 | -0.39517 |
| H | -7.65604 | -6.15529 | -0.43893 |
| H | -5.21353 | -6.21919 | -0.42940 |
| H | -3.27461 | -6.23188 | -0.20165 |
| H | -0.87861 | -6.24828 | -0.17352 |
| H | 1.03519  | -6.26337 | -0.36585 |
| H | 3.43038  | -6.27716 | -0.31941 |
| H | 5.37456  | -6.28480 | -0.23373 |
| H | 7.81595  | -6.24935 | -0.17091 |
| H | 9.04496  | -4.09984 | -0.11518 |
| H | 9.02176  | -1.66500 | -0.08559 |
| H | 9.02883  | 0.77622  | -0.05431 |
| H | 9.05720  | 3.22250  | -0.02278 |
| H | -5.39891 | 6.65470  | -0.21107 |
| H | -2.96578 | 6.66925  | -0.20437 |
| H | -1.04050 | 6.65312  | -0.16652 |
| H | 1.35148  | 6.63866  | -0.12892 |
| H | 3.27789  | 6.63210  | -0.13208 |
| H | 5.70992  | 6.58783  | -0.07392 |
| H | 0.36999  | -2.33875 | 2.84294  |
| H | 1.03458  | 0.04968  | 2.89536  |

|   |          |          |         |
|---|----------|----------|---------|
| H | -3.10359 | 1.20141  | 2.89949 |
| H | -3.76780 | -1.18765 | 2.85002 |
| H | -2.03177 | -2.95717 | 2.82054 |

# Benzene-convex surface of SWCNT, gas

|   |          |          |          |
|---|----------|----------|----------|
| C | 7.73291  | 0.17040  | -0.63602 |
| C | 7.78105  | 0.04060  | 0.75045  |
| C | 7.55075  | -1.19816 | 1.34355  |
| C | 7.27570  | -2.30963 | 0.54928  |
| C | 7.22380  | -2.18102 | -0.83639 |
| C | 7.45365  | -0.94036 | -1.42900 |
| H | 7.08095  | -3.27291 | 1.01178  |
| C | 4.07792  | -1.59435 | 0.70724  |
| C | 3.68378  | -1.50591 | 2.07500  |
| C | 3.04762  | -2.62830 | 2.68487  |
| C | 3.13586  | -3.92197 | 2.07418  |
| C | 3.54372  | -4.01324 | 0.70437  |
| C | 3.84496  | -2.80650 | -0.00756 |
| C | 3.37844  | -5.22272 | 0.00081  |
| C | 3.11899  | -6.39256 | 0.76946  |
| C | 2.72721  | -6.30475 | 2.07815  |
| C | 2.56708  | -5.04093 | 2.71352  |
| C | 2.11939  | -2.41792 | 3.71691  |
| C | 1.27755  | -3.50079 | 4.13313  |
| C | 1.60540  | -4.82365 | 3.77560  |
| C | 3.64175  | -2.75876 | -1.39596 |
| C | 3.13167  | -3.91678 | -2.06947 |
| C | 3.16429  | -5.17257 | -1.43180 |
| C | 1.83091  | -1.08491 | 4.13765  |
| C | 2.67341  | -0.02689 | 3.74215  |
| C | 3.61606  | -0.24093 | 2.69161  |
| C | 4.21979  | 0.88778  | 2.06239  |
| C | 4.60535  | 0.79942  | 0.71654  |
| C | 4.39774  | -0.41734 | 0.00501  |
| C | 4.19376  | -0.36915 | -1.40518 |
| C | 3.67851  | -1.50034 | -2.06699 |
| C | 2.36510  | 1.31086  | 4.13160  |
| C | 3.22940  | 2.38866  | 3.74746  |
| C | 4.17419  | 2.17361  | 2.69450  |
| C | 4.83639  | 3.26961  | 2.10728  |
| C | 5.24763  | 3.17438  | 0.71994  |
| C | 4.96094  | 1.99325  | 0.00855  |
| C | 4.75867  | 2.04187  | -1.40675 |
| C | 4.20711  | 0.89484  | -2.06515 |
| C | 2.96273  | 3.69763  | 4.19422  |
| C | 3.87904  | 4.71642  | 3.81000  |
| C | 4.78294  | 4.51011  | 2.80254  |
| C | 4.83707  | 3.27338  | -2.08672 |
| C | 5.44025  | 4.36096  | -1.39413 |
| C | 5.63911  | 4.31255  | -0.03996 |
| C | 3.44255  | 1.07196  | -3.22868 |
| C | 3.22902  | 2.39744  | -3.73003 |
| C | 4.04419  | 3.45765  | -3.28588 |
| C | 2.89832  | -1.32053 | -3.24834 |
| C | 2.66893  | -0.01680 | -3.73090 |
| C | 1.46580  | 0.26099  | -4.44622 |
| C | 1.07267  | 1.61925  | -4.63884 |
| C | 2.02293  | 2.67590  | -4.44777 |
| C | 1.65244  | 4.00999  | -4.70767 |
| C | 2.65308  | 5.00832  | -4.53821 |
| C | 3.80743  | 4.74182  | -3.85246 |
| C | -0.29174 | 1.93394  | -4.74101 |
| C | -0.70311 | 3.30422  | -4.65300 |
| C | 0.24423  | 4.33470  | -4.81349 |
| C | 0.53401  | -0.77546 | -4.65501 |
| C | -0.85313 | -0.45531 | -4.75926 |
| C | -1.25997 | 0.88941  | -4.65172 |
| C | -2.55384 | 1.18710  | -4.12796 |
| C | -2.84176 | 2.52027  | -3.70882 |
| C | -2.00039 | 3.60257  | -4.12781 |
| C | -2.32779 | 4.92597  | -3.77215 |
| C | -1.47535 | 5.95908  | -4.25348 |
| C | -0.23444 | 5.67382  | -4.75609 |
| C | -3.77120 | 2.73238  | -2.67801 |

C -3.85741 4.02689 -2.06864  
 C -3.28760 5.14478 -2.70885  
 C -3.39654 0.12986 -3.73083  
 C -4.34198 0.34567 -2.68322  
 C -4.41106 1.61178 -2.06903  
 C -4.81831 1.70446 -0.70388  
 C -4.57359 2.91438 0.01169  
 C -4.26544 4.11978 -0.69985  
 C -4.09663 5.32825 0.00390  
 C -3.83434 6.49745 -0.76430  
 C -3.44432 6.40881 -2.07346  
 C -4.36711 2.86452 1.39948  
 C -3.85332 4.02076 2.07299  
 C -3.88420 5.27701 1.43647  
 C -5.14180 0.52709 -0.00072  
 C -4.93180 0.47637 1.41022  
 C -4.40536 1.60511 2.06885  
 C -3.62230 1.42328 3.24821  
 C -2.82391 2.50603 3.72357  
 C -3.06858 3.83853 3.25560  
 C -2.32824 4.91567 3.78109  
 C -2.64838 6.21855 3.30613  
 C -3.39902 6.39291 2.17473  
 C -1.64152 2.23254 4.42912  
 C -0.70508 3.29219 4.66390  
 C -1.10753 4.63330 4.50885  
 C -3.39195 0.11866 3.72750  
 C -2.18973 -0.15961 4.44447  
 C -1.25863 0.87672 4.65652  
 C 0.12832 0.55691 4.76555  
 C 1.09125 1.60294 4.64378  
 C 0.68539 2.97166 4.77297  
 C 1.64841 3.99844 4.72521  
 C 1.18695 5.33286 4.90227  
 C -0.14301 5.63959 4.79733  
 C 0.53570 -0.78773 4.65800  
 C -0.02094 -3.20283 4.65573  
 C -0.43262 -1.83255 4.74363  
 C -1.79666 -1.51782 4.63722  
 C -2.74662 -2.57406 4.44470  
 C -3.95256 -2.29496 3.72697  
 C -4.16743 -0.96929 3.22639  
 C -4.93786 -0.79044 2.06674  
 C -5.49224 -1.93734 1.40971  
 C -5.70278 -1.88640 -0.00497  
 C -5.35230 -0.69082 -0.71363  
 C -4.95188 -0.78189 -2.05641  
 C -4.90273 -2.06793 -2.68731  
 C -3.95467 -2.28441 -3.73741  
 C -3.08914 -1.20790 -4.12051  
 C -1.81615 -1.50091 -4.63453  
 C -1.41101 -2.86973 -4.76359  
 C -0.02040 -3.19080 -4.65692  
 C 0.91694 -2.13120 -4.42622  
 C 2.10044 -2.40423 -3.72225  
 C 2.34541 -3.73600 -3.25180  
 C 0.75140 -5.85734 4.25316  
 C -0.49035 -5.57257 4.75395  
 C -0.96877 -4.23332 4.81283  
 C -2.37666 -3.90817 4.70539  
 C -3.37791 -4.90600 4.53693  
 C -4.53237 -4.63895 3.85185  
 C -4.76841 -3.35491 3.28451  
 C -5.56339 -3.17033 2.08730  
 C -6.16211 -4.26038 1.39483  
 C -6.36304 -4.21191 0.04170  
 C -5.98029 -3.07000 -0.71687  
 C -5.56664 -3.16407 -2.10226  
 C -5.51411 -4.40424 -2.79880  
 C -4.60798 -4.61117 -3.80356  
 C -3.68861 -3.59350 -4.18401  
 C -2.37450 -3.89594 -4.71371  
 C -1.91386 -5.23100 -4.88891  
 C -0.58395 -5.53818 -4.78503  
 C 0.38176 -4.53188 -4.50016

C 1.60389 -4.81372 -3.77451  
 C 1.92501 -6.11615 -3.29852  
 C 2.67799 -6.28931 -2.16850  
 H -1.75939 6.99775 -4.12626  
 H 0.42499 6.49587 -5.01115  
 H 2.46151 6.02610 -4.85943  
 H 4.49390 5.55693 -3.65230  
 H 5.65200 5.28627 -1.91822  
 H 6.00213 5.20119 0.46473  
 H 5.38662 5.34593 2.46662  
 H 3.79519 5.70872 4.23897  
 H 1.90033 6.14134 5.01582  
 H -0.44164 6.68153 4.82978  
 H -2.20783 7.08984 3.77780  
 H -3.52936 7.39656 1.78553  
 H -3.83807 7.47080 -0.28647  
 H -3.15051 7.31456 -2.59216  
 H 1.48356 -6.98800 -3.76832  
 H 2.80874 -7.29266 -1.77861  
 H 3.12573 -7.36609 0.29196  
 H 2.43525 -7.21121 2.59672  
 H 1.03490 -6.89593 4.12394  
 H -1.15070 -6.39489 5.00574  
 H -3.18739 -5.92345 4.85982  
 H -5.22052 -5.45317 3.65412  
 H -6.36775 -5.18731 1.91830  
 H -6.72020 -5.10219 -0.46400  
 H -6.12215 -5.23827 -2.46664  
 H -4.52582 -5.60264 -4.23479  
 H -2.62768 -6.03943 -5.00000  
 H -0.28601 -6.58037 -4.81581  
 H 7.57566 -1.29609 2.42449  
 H 6.98943 -3.04355 -1.45311  
 H 7.39988 -6.03638 -2.50859  
 H 7.89437 1.14114 -1.09604  
 H 7.98002 0.91118 1.36888

# Ethane-concave surface of SWCNT, gas

C -4.28317 2.29815 4.26429  
 C -4.27525 3.47226 3.41577  
 C -3.05597 3.88995 2.84713  
 C -1.81619 3.39409 3.36856  
 C -1.82410 2.25471 4.18867  
 C -3.07148 1.61566 4.48869  
 C -5.46941 4.03111 2.87928  
 C -5.46529 4.67954 1.67391  
 C -4.26655 4.81645 0.91890  
 C -3.05163 4.56902 1.58762  
 C -1.80750 4.72958 0.89409  
 C -1.80712 4.78738 -0.50854  
 C -3.05062 4.68164 -1.21408  
 C -4.26616 4.87413 -0.52888  
 C -0.57347 4.54954 1.58796  
 C -0.57777 3.87041 2.84330  
 C -3.05354 4.10523 -2.52380  
 C -4.27159 3.73227 -3.12502  
 C -5.46684 4.24525 -2.54685  
 C -5.46419 4.79642 -1.29391  
 C -1.81254 3.65578 -3.08251  
 C -0.57552 4.09173 -2.52038  
 C -0.57259 4.66603 -1.21383  
 C 0.64713 4.79060 -0.51924  
 C 0.64684 4.72987 0.90696  
 C -4.27671 2.63021 -4.06574  
 C -3.06301 1.97149 -4.34477  
 C -1.81740 2.58709 -3.99253  
 C -0.58517 1.95611 -4.33790  
 C 0.63666 2.57630 -4.01057  
 C 0.64155 3.66393 -3.08670  
 C 1.87846 4.07104 -2.50365  
 C 1.88135 4.63483 -1.21826  
 C 1.88075 4.51350 1.59049  
 C 3.12497 4.71740 0.90864  
 C 3.12532 4.78080 -0.52113

C 4.34122 4.69927 -1.22785  
 C 4.33813 4.11921 -2.55538  
 C 3.11931 3.65657 -3.08916  
 C 3.11443 2.56563 -4.01493  
 C 1.86855 1.92832 -4.32407  
 C 4.32805 1.95730 -4.39100  
 C 5.52854 2.66190 -4.09378  
 C 5.53336 3.70570 -3.20820  
 C 4.34085 4.57248 1.60516  
 C 5.53961 4.83074 0.88243  
 C 5.53988 4.89260 -0.48492  
 C 4.33686 3.87909 2.87740  
 C 3.11666 3.37833 3.37300  
 C 1.87668 3.84430 2.82462  
 C 0.63842 3.39419 3.37282  
 C 4.32133 0.55524 -4.75668  
 C 3.10096 -0.14799 -4.72693  
 C 1.86189 0.57070 -4.68101  
 C 0.62342 -0.13564 -4.72672  
 C -0.59191 0.57643 -4.70276  
 C -1.83047 -0.13120 -4.71673  
 C -3.06956 0.58907 -4.71464  
 C -4.28964 -0.11007 -4.80288  
 C -5.48365 0.66427 -4.83282  
 C -5.47738 1.98563 -4.47661  
 C 0.61490 -1.53916 -4.46716  
 C -0.60843 -2.18306 -4.19505  
 C -1.83857 -1.51156 -4.46236  
 C -3.08555 -2.17093 -4.21088  
 C -4.29713 -1.53598 -4.54606  
 C 0.63024 2.23604 4.20680  
 C -0.59378 1.59506 4.48303  
 C 1.84528 -2.19598 -4.16746  
 C 3.09230 -1.55472 -4.46477  
 C 3.10847 2.21736 4.20964  
 C 1.86035 1.56226 4.46968  
 C 4.30468 -2.23490 -4.23690  
 C 5.50663 -1.56063 -4.59142  
 C 5.51487 -0.21508 -4.84251  
 C 4.32025 1.57763 4.53710  
 C 5.52365 2.29604 4.28991  
 C 5.53167 3.40680 3.49003  
 C -0.60463 0.19089 4.73801  
 C 0.60909 -0.52359 4.70906  
 C 1.84949 0.18123 4.72216  
 C 3.08662 -0.54238 4.71716  
 C 4.30886 0.15289 4.80160  
 C -3.08228 0.20760 4.74397  
 C -1.84472 -0.51306 4.69090  
 C -1.85497 -1.86857 4.32559  
 C -0.62483 -2.51905 4.01084  
 C 0.59837 -1.90202 4.33955  
 C 1.82872 -2.53628 3.99524  
 C 3.07581 -1.92539 4.34970  
 C 4.28713 -2.59005 4.07533  
 C 5.48930 -1.94915 4.48731  
 C 5.49985 -0.62584 4.83682  
 C -0.63218 -3.60691 3.08680  
 C 0.58438 -4.03766 2.52117  
 C 1.82163 -3.60554 3.08624  
 C 3.06200 -4.06210 2.53273  
 C 4.27977 -3.69455 3.13769  
 C -5.48542 1.62563 4.62173  
 C -5.49565 0.27902 4.86636  
 C -4.30396 -0.49328 4.77079  
 C -4.31443 -1.89195 4.39287  
 C -3.10240 -2.50074 4.01229  
 C -3.10952 -3.58893 3.08329  
 C -1.86925 -4.01082 2.50198  
 C -1.87134 -4.57899 1.21837  
 C -0.63622 -4.74230 0.52184  
 C 0.58237 -4.61753 1.21819  
 C 1.81834 -4.74621 0.51626  
 C 3.06039 -4.64104 1.22454  
 C 4.27731 -4.83727 0.54307

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.47315  | -4.76647 | 1.31219  |
| C | 5.47423  | -4.21544 | 2.56514  |
| C | -0.63195 | -4.68854 | -0.90480 |
| C | 0.59010  | -4.51017 | -1.58384 |
| C | 1.82220  | -4.69033 | -0.88676 |
| C | 3.06859  | -4.52304 | -1.57512 |
| C | 4.28176  | -4.77292 | -0.90432 |
| C | -5.51683 | -2.59095 | 4.09065  |
| C | -5.52418 | -3.63000 | 3.19947  |
| C | -4.32954 | -4.04631 | 2.54754  |
| C | -4.33224 | -4.62955 | 1.22173  |
| C | -3.11436 | -4.72133 | 0.51898  |
| C | -3.11064 | -4.66718 | -0.91116 |
| C | -1.86414 | -4.47168 | -1.59166 |
| C | -1.85661 | -3.79806 | -2.82321 |
| C | -0.61703 | -3.34398 | -3.36493 |
| C | 0.59765  | -3.82305 | -2.83513 |
| C | 1.83651  | -3.33856 | -3.35140 |
| C | 3.07584  | -3.83467 | -2.82923 |
| C | 4.29615  | -3.41161 | -3.39174 |
| C | 5.48954  | -3.97160 | -2.85499 |
| C | 5.48272  | -4.62849 | -1.65417 |
| C | -5.53024 | -4.82025 | 0.47724  |
| C | -5.52662 | -4.76809 | -0.89037 |
| C | -4.32474 | -4.52163 | -1.61169 |
| C | -4.31584 | -3.83687 | -2.88803 |
| C | -3.09454 | -3.33292 | -3.37608 |
| C | -5.50759 | -3.37509 | -3.51548 |
| C | -5.49845 | -2.26408 | -4.31564 |
| C | 0.33834  | -1.23317 | -0.41386 |
| C | -1.08180 | -1.25512 | 0.14659  |
| H | -1.07538 | -1.38389 | 1.23512  |
| H | 6.43356  | -2.47855 | 4.42500  |
| H | 6.45218  | -0.14860 | 5.03984  |
| H | 6.46947  | 1.90615  | 4.64924  |
| H | 6.48371  | 3.86184  | 3.24027  |
| H | 6.48834  | 4.87356  | 1.40571  |
| H | 6.48896  | 4.98254  | -1.00145 |
| H | 6.48364  | 4.14530  | -2.92619 |
| H | 6.47519  | 2.30709  | -4.48580 |
| H | 6.46698  | 0.27791  | -5.00426 |
| H | 6.45226  | -2.09042 | -4.56225 |
| H | 6.44054  | -3.78789 | -3.34235 |
| H | 6.42815  | -4.94390 | -1.22712 |
| H | 6.41999  | -5.05150 | 0.86702  |
| H | 6.42213  | -4.08230 | 3.07451  |
| H | -6.41914 | 3.85245  | 3.37101  |
| H | -6.41159 | 4.99444  | 1.24840  |
| H | -6.41107 | 5.07589  | -0.84537 |
| H | -6.41609 | 4.10636  | -3.05214 |
| H | -6.42415 | 2.50989  | -4.40845 |
| H | -6.43497 | 0.18429  | -5.03460 |
| H | -6.44026 | -1.88236 | -4.69379 |
| H | -6.45667 | -3.84360 | -3.27976 |
| H | -6.47465 | -4.80700 | -1.41539 |
| H | -6.48142 | -4.90002 | 0.99167  |
| H | -6.47579 | -4.06482 | 2.91453  |
| H | -6.46267 | -2.23569 | 4.48421  |
| H | -6.44809 | -0.21274 | 5.02989  |
| H | -6.42983 | 2.15788  | 4.59860  |
| H | -1.60877 | -0.32218 | -0.07331 |
| H | -1.67010 | -2.07405 | -0.28132 |
| H | 0.33719  | -1.15700 | -1.50769 |
| H | 0.90240  | -0.38146 | -0.02277 |
| H | 0.88750  | -2.14170 | -0.14474 |

#### Ethane-graphene, gas

|   |         |          |          |
|---|---------|----------|----------|
| C | 7.18695 | 4.44643  | -0.05134 |
| C | 5.74679 | 4.47494  | -0.05785 |
| C | 5.02213 | 3.25296  | -0.07326 |
| C | 5.72387 | 2.02003  | -0.08255 |
| C | 7.16376 | 2.01509  | -0.07480 |
| C | 7.86250 | 3.27750  | -0.05908 |
| C | 5.01101 | 0.80396  | -0.09860 |
| C | 5.71668 | -0.42802 | -0.10644 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 7.15366  | -0.42258 | -0.09729 |
| C | 7.84010  | 0.81834  | -0.08195 |
| C | 5.01416  | -1.65172 | -0.12247 |
| C | 3.57633  | -1.64801 | -0.13342 |
| C | 2.87014  | -0.42949 | -0.12592 |
| C | 3.57881  | 0.80982  | -0.10722 |
| C | 2.87763  | 2.03137  | -0.09615 |
| C | 3.59786  | 3.26548  | -0.07841 |
| C | 5.73157  | -2.87508 | -0.12874 |
| C | 7.16316  | -2.85823 | -0.11886 |
| C | 7.84045  | -1.63231 | -0.10367 |
| C | 2.86837  | -2.88580 | -0.15137 |
| C | 3.57803  | -4.11730 | -0.15663 |
| C | 5.04281  | -4.12372 | -0.14508 |
| C | 5.78709  | -5.29589 | -0.15066 |
| C | 7.19298  | -5.27669 | -0.14057 |
| C | 7.87271  | -4.08667 | -0.12514 |
| C | 1.43720  | -0.42429 | -0.13848 |
| C | 0.72704  | -1.64261 | -0.15966 |
| C | 1.44053  | -2.88090 | -0.16569 |
| C | 0.73096  | -4.10892 | -0.18689 |
| C | 1.46133  | -5.29850 | -0.18804 |
| C | 2.84305  | -5.30155 | -0.17346 |
| C | 1.44439  | 2.03658  | -0.10179 |
| C | 0.73346  | 0.81762  | -0.12349 |
| C | -0.70741 | -1.63845 | -0.17265 |
| C | -1.42809 | -2.87239 | -0.19554 |
| C | -0.72636 | -4.10434 | -0.20487 |
| C | -1.40966 | -0.41613 | -0.14659 |
| C | -0.69862 | 0.82176  | -0.12500 |
| C | -2.84287 | -0.41271 | -0.14057 |
| C | -3.55636 | -1.62697 | -0.16176 |
| C | -2.85566 | -2.86895 | -0.19191 |
| C | -3.57292 | -4.09599 | -0.21047 |
| C | -2.84517 | -5.28456 | -0.22740 |
| C | -1.46345 | -5.28958 | -0.22299 |
| C | 2.90927  | 4.50414  | -0.06586 |
| C | 1.45217  | 4.50584  | -0.06513 |
| C | 0.73869  | 3.27736  | -0.08305 |
| C | -0.68942 | 3.28142  | -0.08042 |
| C | -1.40242 | 2.04471  | -0.09978 |
| C | -2.83574 | 2.04787  | -0.09463 |
| C | -3.54421 | 0.83062  | -0.11331 |
| C | -4.97642 | 0.83319  | -0.10732 |
| C | -5.68944 | -0.39447 | -0.12832 |
| C | -4.99427 | -1.62212 | -0.15614 |
| C | -5.71899 | -2.84103 | -0.17931 |
| C | -5.03771 | -4.09355 | -0.20862 |
| C | -7.12637 | -0.38050 | -0.12244 |
| C | -7.82037 | -1.58593 | -0.14524 |
| C | -7.15044 | -2.81563 | -0.17419 |
| C | -7.86739 | -4.03957 | -0.19923 |
| C | -7.19480 | -5.23336 | -0.22869 |
| C | -5.78904 | -5.26098 | -0.23365 |
| C | -7.80542 | 0.86426  | -0.09426 |
| C | -7.12197 | 2.05681  | -0.07414 |
| C | -5.68206 | 2.05325  | -0.08113 |
| C | -4.97298 | 3.28189  | -0.06207 |
| C | -3.54863 | 3.28605  | -0.06919 |
| C | -2.85273 | 4.52060  | -0.05098 |
| C | -1.39565 | 4.51397  | -0.05781 |
| C | -0.65817 | 5.69997  | -0.04160 |
| C | 0.72164  | 5.69602  | -0.04529 |
| C | -5.69035 | 4.50796  | -0.03609 |
| C | -7.13067 | 4.48790  | -0.02810 |
| C | -7.81316 | 3.32316  | -0.04615 |
| C | -4.97654 | 5.70600  | -0.01865 |
| C | -3.59319 | 5.71075  | -0.02608 |
| C | 5.04009  | 5.67728  | -0.04900 |
| C | 3.65679  | 5.69015  | -0.05275 |
| C | -0.74155 | -2.23262 | 3.11140  |
| C | -0.07786 | -0.87745 | 3.33548  |
| H | -0.67831 | -0.24664 | 3.99658  |
| H | -7.65465 | 5.43931  | -0.00681 |
| H | 7.71659  | 5.39485  | -0.03925 |

|   |          |          |          |
|---|----------|----------|----------|
| H | -8.90739 | -1.57498 | -0.14113 |
| H | -8.89257 | 0.86555  | -0.08928 |
| H | -8.89919 | 3.31182  | -0.04013 |
| H | -8.95287 | -4.00897 | -0.19506 |
| H | -7.74312 | -6.16950 | -0.24886 |
| H | -5.30158 | -6.22770 | -0.25917 |
| H | -3.35627 | -6.23913 | -0.24045 |
| H | -0.96200 | -6.24871 | -0.23240 |
| H | 0.95436  | -6.25463 | -0.20135 |
| H | 3.34846  | -6.25925 | -0.17589 |
| H | 5.29384  | -6.25989 | -0.16382 |
| H | 7.73572  | -6.21628 | -0.14553 |
| H | 8.95833  | -4.06254 | -0.11757 |
| H | 8.92750  | -1.62781 | -0.09667 |
| H | 8.92724  | 0.81324  | -0.07563 |
| H | 8.94844  | 3.25978  | -0.05353 |
| H | -5.52066 | 6.64600  | 0.00140  |
| H | -3.08772 | 6.66794  | -0.01108 |
| H | -1.16158 | 6.65813  | -0.02463 |
| H | 1.23067  | 6.65123  | -0.03024 |
| H | 3.15699  | 6.65042  | -0.04507 |
| H | 5.58979  | 6.61417  | -0.03823 |
| H | -0.88868 | -2.76311 | 4.05647  |
| H | -1.72081 | -2.12076 | 2.63480  |
| H | -0.13172 | -2.86992 | 6.62272  |
| H | 0.91111  | -0.98982 | 3.78818  |
| H | 0.05046  | -0.33749 | 2.39272  |

#### Ethane-convex surface of SWCNT, gas

|   |          |         |          |
|---|----------|---------|----------|
| C | -4.31595 | 3.08413 | 3.55593  |
| C | -4.32751 | 3.98053 | 2.41782  |
| C | -3.11560 | 4.24288 | 1.74936  |
| C | -1.86837 | 3.92741 | 2.38092  |
| C | -1.85656 | 3.06092 | 3.48500  |
| C | -3.09315 | 2.50956 | 3.95497  |
| C | -5.53037 | 4.35697 | 1.75639  |
| C | -5.53788 | 4.65603 | 0.42068  |
| C | -4.34281 | 4.60162 | -0.35097 |
| C | -3.12332 | 4.55549 | 0.35252  |
| C | -1.88323 | 4.53770 | -0.36585 |
| C | -1.88607 | 4.22930 | -1.73556 |
| C | -3.12909 | 3.93156 | -2.38337 |
| C | -4.34572 | 4.27848 | -1.76358 |
| C | -0.64631 | 4.55999 | 0.34348  |
| C | -0.63839 | 4.25656 | 1.73737  |
| C | -3.12626 | 3.04059 | -3.50325 |
| C | -4.34076 | 2.51231 | -3.98364 |
| C | -5.54166 | 3.13959 | -3.54733 |
| C | -5.54408 | 3.99187 | -2.47623 |
| C | -1.88059 | 2.47989 | -3.93826 |
| C | -0.64846 | 3.05836 | -3.51036 |
| C | -0.65154 | 3.94547 | -2.39232 |
| C | 0.56788  | 4.25709 | -1.75844 |
| C | 0.57035  | 4.56861 | -0.36637 |
| C | -4.33281 | 1.20761 | -4.61367 |
| C | -3.11098 | 0.51465 | -4.72256 |
| C | -1.87278 | 1.21575 | -4.54880 |
| C | -0.63272 | 0.53309 | -4.72965 |
| C | 0.58151  | 1.23166 | -4.57716 |
| C | 0.57362  | 2.51650 | -3.95602 |
| C | 1.80624  | 3.07217 | -3.49912 |
| C | 1.80333  | 3.94500 | -2.40005 |
| C | 1.80747  | 4.57150 | 0.34309  |
| C | 3.04704  | 4.60615 | -0.37547 |
| C | 3.04491  | 4.28497 | -1.77044 |
| C | 4.26113  | 4.03926 | -2.43740 |
| C | 4.26482  | 3.13668 | -3.57081 |
| C | 3.05186  | 2.53937 | -3.96635 |
| C | 3.05980  | 1.25134 | -4.58958 |
| C | 1.82178  | 0.54095 | -4.72300 |
| C | 4.28086  | 0.58313 | -4.80565 |
| C | 5.47295  | 1.35365 | -4.69796 |
| C | 5.46518  | 2.58562 | -4.10136 |
| C | 4.26555  | 4.67657 | 0.32767  |

C 5.45967 4.74652 -0.44410  
 C 5.45737 4.43918 -1.77803  
 C 4.27408 4.36139 1.74225  
 C 3.06355 3.99724 2.36395  
 C 1.81563 4.27065 1.71461  
 C 0.58618 3.96946 2.37299  
 C 4.29253 -0.86559 -4.80266  
 C 3.08250 -1.55244 -4.58325  
 C 1.83333 -0.86258 -4.71936  
 C 0.60452 -1.57243 -4.56932  
 C -0.62080 -0.89427 -4.72521  
 C -1.84948 -1.59608 -4.53975  
 C -3.09894 -0.91651 -4.71813  
 C -4.30918 -1.62878 -4.60519  
 C -5.51344 -0.90564 -4.83481  
 C -5.52496 0.46318 -4.83884  
 C 0.61739 -2.85423 -3.94143  
 C -0.59539 -3.41318 -3.49135  
 C -1.83673 -2.85671 -3.92195  
 C -3.07309 -3.43518 -3.48388  
 C -4.29593 -2.92561 -3.96723  
 C 0.59797 3.08844 3.49582  
 C -0.61473 2.52830 3.94445  
 C 1.85863 -3.38853 -3.48315  
 C 3.09535 -2.83796 -3.95454  
 C 3.07572 3.11233 3.48850  
 C 1.83967 2.53292 3.92635  
 C 4.31791 -3.41435 -3.55791  
 C 5.50888 -2.84705 -4.09261  
 C 5.49664 -1.61692 -4.69321  
 C 4.29887 2.60689 3.97142  
 C 5.48903 3.25263 3.53232  
 C 5.47698 4.09928 2.45695  
 C -0.60131 1.24627 4.57153  
 C 0.62450 0.56871 4.72698  
 C 1.85287 1.27146 4.54257  
 C 3.10272 0.59210 4.71990  
 C 4.31261 1.30513 4.60788  
 C -3.07953 1.22450 4.58414  
 C -1.82976 0.53559 4.72077  
 C -1.81717 -0.86817 4.72360  
 C -0.57654 -1.55808 4.57675  
 C 0.63716 -0.85877 4.72954  
 C 1.87756 -1.54057 4.54741  
 C 3.11541 -0.83913 4.72202  
 C 4.33755 -1.53149 4.61207  
 C 5.52937 -0.78685 4.83813  
 C 5.51722 0.58208 4.83618  
 C -0.56813 -2.84276 3.95479  
 C 0.65390 -3.38332 3.50776  
 C 1.88574 -2.80404 3.93549  
 C 3.13148 -3.36394 3.50021  
 C 4.34587 -2.83556 3.98081  
 C -5.50713 2.51540 4.08909  
 C -5.49406 1.28623 4.69094  
 C -4.28915 0.53655 4.80293  
 C -4.27613 -0.91250 4.80774  
 C -3.05459 -1.57973 4.59091  
 C -3.04592 -2.86804 3.96811  
 C -1.80028 -3.40002 3.49938  
 C -1.79743 -4.27437 2.40122  
 C -0.56247 -4.58878 1.75953  
 C 0.65661 -4.27185 2.39083  
 C 1.89111 -4.55528 1.73381  
 C 3.13419 -4.25527 2.38072  
 C 4.35092 -4.60216 1.76132  
 C 5.54926 -4.31471 2.47340  
 C 5.54685 -3.46224 3.54428  
 C -0.56614 -4.90746 0.36810  
 C 0.64978 -4.89936 -0.34346  
 C 1.88772 -4.86921 0.36549  
 C 3.12751 -4.88379 -0.35333  
 C 4.34749 -4.92689 0.34928  
 C -5.46746 -1.68465 4.70279  
 C -5.45908 -2.91712 4.10725

C -4.25893 -3.46672 3.57488  
 C -4.25600 -4.36882 2.44110  
 C -3.04033 -4.61427 1.77308  
 C -3.04394 -4.93362 0.37790  
 C -1.80448 -4.90217 -0.34099  
 C -1.81321 -4.59600 -1.71107  
 C -0.58353 -4.29574 -2.36965  
 C 0.64077 -4.58857 -1.73663  
 C 1.87027 -4.25710 -2.38029  
 C 3.11847 -4.57273 -1.75035  
 C 4.32993 -4.31067 -2.41983  
 C 5.53348 -4.68566 -1.75902  
 C 5.54210 -4.98190 -0.42279  
 C -5.45315 -4.76709 1.78218  
 C -5.45680 -5.07171 0.44776  
 C -4.26325 -5.00124 -0.32449  
 C -4.27203 -4.68444 -1.73836  
 C -3.06118 -4.32031 -2.35954  
 C -5.47465 -4.42153 -2.45269  
 C -5.48633 -3.57462 -3.52794  
 C 0.37166 7.89421 0.58375  
 C -0.55988 7.87230 -0.62530  
 H 1.42155 7.88247 0.27674  
 H 6.48281 -1.29853 4.90772  
 H 6.46139 1.11069 4.90382  
 H 6.44120 2.99626 3.98310  
 H 6.42025 4.48635 2.08847  
 H 6.40822 4.94189 0.04422  
 H 6.40433 4.40083 -2.30542  
 H 6.41048 3.09194 -3.94087  
 H 6.42365 0.92273 -4.99242  
 H 6.44012 -1.17211 -4.98984  
 H 6.46207 -3.33809 -3.93183  
 H 6.47902 -4.63538 -2.28768  
 H 6.49412 -5.15698 0.06563  
 H 6.49881 -4.68677 2.10576  
 H 6.49490 -3.18627 3.99249  
 H -6.47622 4.30678 2.28429  
 H -6.48944 4.83282 -0.06790  
 H -6.49405 4.36430 -2.10889  
 H -6.48970 2.86422 -3.99595  
 H -6.47817 0.97516 -4.90949  
 H -6.45783 -1.43388 -4.90189  
 H -6.43849 -3.31768 -3.97854  
 H -6.41807 -4.80848 -2.08404  
 H -6.40542 -5.26512 -0.04010  
 H -6.39914 -4.72866 2.31051  
 H -6.40384 -3.42505 3.94903  
 H -6.41800 -1.25497 4.99895  
 H -6.43750 0.84034 4.98600  
 H -6.46097 3.00447 3.92587  
 H 0.21103 8.79073 1.18921  
 H 0.20788 7.02639 1.22989  
 H -1.60784 7.80752 -0.31799  
 H -0.44414 8.77680 -1.22912  
 H -0.35366 7.01451 -1.27264

# Methane-concave surface of SWCNT, gas

C -4.30989 1.77922 -4.47111  
 C -4.30664 0.36520 -4.78758  
 C -3.08841 -0.33982 -4.72954  
 C -1.84735 0.37652 -4.70685  
 C -1.85053 1.74674 -4.40176  
 C -3.09498 2.39822 -4.11707  
 C -5.50227 -0.40447 -4.85012  
 C -5.49899 -1.73998 -4.55016  
 C -4.30021 -2.40311 -4.16447  
 C -3.08512 -1.73592 -4.41507  
 C -1.84111 -2.36816 -4.08782  
 C -1.83871 -3.47373 -3.22297  
 C -3.08112 -3.94421 -2.68544  
 C -4.29811 -3.54338 -3.27076  
 C -0.60772 -1.72706 -4.40847  
 C -0.61092 -0.33493 -4.72228

C 0.61241 -2.36346 -4.10721  
 C 0.61480 -3.48930 -3.22961  
 C -0.60290 -3.93860 -2.68150  
 C -0.60111 -4.57407 -1.40353  
 C -1.83629 -4.71893 -0.70331  
 C -3.08000 -4.57732 -1.40251  
 C -4.29615 -4.79433 -0.72584  
 C -5.49399 -4.68096 -1.48649  
 C -5.49480 -4.07729 -2.71498  
 C -1.83629 -4.71934 0.70064  
 C -3.08000 -4.57813 1.39991  
 C -4.29615 -4.79476 0.72313  
 C -0.60111 -4.57488 1.40094  
 C 0.61789 -4.73443 0.71260  
 C 0.61789 -4.73401 -0.71529  
 C 1.85244 -4.54568 -1.40615  
 C 1.85110 -3.92374 -2.66465  
 C 3.09287 -3.48611 -3.23209  
 C 3.09018 -2.35938 -4.11397  
 C 1.84575 -1.70743 -4.39738  
 C 1.84279 -0.33786 -4.70544  
 C 0.60651 0.37376 -4.72351  
 C 0.60336 1.76692 -4.41374  
 C -0.61710 2.40301 -4.11226  
 C -0.60290 -3.94014 2.67926  
 C -1.83871 -3.47558 3.22100  
 C -3.08112 -3.94576 2.68321  
 C -4.29812 -3.54527 3.26876  
 C -5.49480 -4.07887 2.71268  
 C -5.49399 -4.68183 1.48384  
 C 3.09658 -4.72387 -0.71675  
 C 3.09658 -4.72429 0.71408  
 C 1.85243 -4.54650 1.40357  
 C 1.85110 -3.92527 2.66243  
 C 0.61480 -3.49116 3.22763  
 C 0.61241 -2.36582 4.10589  
 C -0.60772 -1.72960 4.40751  
 C -1.84111 -2.37052 4.08650  
 C -3.08512 -1.73846 4.41411  
 C -4.30021 -2.40551 4.16313  
 C 4.31274 -4.61274 -1.41896  
 C 4.31098 -3.97365 -2.71917  
 C 1.84575 -1.70997 4.39644  
 C 3.09018 -2.36176 4.11266  
 C 3.09287 -3.48798 3.23013  
 C 4.31098 -3.97523 2.71694  
 C 4.31273 -4.61357 1.41636  
 C 5.51083 -4.84321 0.68302  
 C 5.51083 -4.84280 -0.68576  
 C 4.30505 -1.74111 -4.46947  
 C 5.50407 -2.45840 -4.19879  
 C 5.50712 -3.53533 -3.35388  
 C 4.30211 -0.32733 -4.78699  
 C 3.08408 0.37809 -4.73023  
 C 3.08101 1.77480 -4.41835  
 C 1.83693 2.40799 -4.09316  
 C 4.30505 -1.74370 4.46851  
 C 5.50407 -2.46084 4.19744  
 C 5.50712 -3.53729 3.35191  
 C 4.29615 2.44147 -4.16646  
 C 5.49496 1.77765 -4.55085  
 C 5.49798 0.44193 -4.84995  
 C -0.61957 3.52571 -3.23117  
 C 0.59862 3.97363 -2.68265  
 C 1.83465 3.51188 -3.22606  
 C 3.07675 3.98079 -2.68591  
 C 4.29393 3.58081 -3.27140  
 C -3.09754 3.52355 -3.23324  
 C -1.85564 3.95934 -2.66522  
 C -1.85697 4.57659 -1.40437  
 C -0.62220 4.75863 -0.71244  
 C 0.59723 4.60137 -1.40078  
 C 1.83208 4.74759 -0.70056  
 C 3.07547 4.60969 -1.40057  
 C 4.29152 4.82568 -0.72317

C 5.48941 4.71412 -1.48401  
 C 5.49052 4.11319 -2.71386  
 C -0.62220 4.75821 0.71514  
 C 0.59724 4.60055 1.40338  
 C 1.83208 4.74717 0.70325  
 C 3.07547 4.60886 1.40318  
 C 4.29152 4.82525 0.72590  
 C -5.50909 2.49569 -4.19866  
 C -5.51192 3.57163 -3.35249  
 C -4.31543 4.00962 -2.71808  
 C -4.31679 4.64651 -1.41667  
 C -3.10051 4.75590 -0.71427  
 C -3.10051 4.75548 0.71697  
 C -1.85697 4.57577 1.40697  
 C -1.85563 3.95780 2.66747  
 C -0.61957 3.52384 3.23317  
 C 0.59863 3.97207 2.68490  
 C 1.83466 3.51001 3.22804  
 C 3.07675 3.97922 2.68816  
 C 4.29394 3.57890 3.27342  
 C 5.49052 4.11159 2.71617  
 C 5.48941 4.71323 1.48667  
 C -0.61709 2.40063 4.11361  
 C 0.60337 1.76437 4.41474  
 C 1.83694 2.40562 4.09451  
 C 3.08101 1.77224 4.41935  
 C 4.29615 2.43905 4.16783  
 C -5.51467 4.87665 -0.68301  
 C -5.51467 4.87625 0.68579  
 C -4.31678 4.64569 1.41932  
 C -4.31542 4.00805 2.72036  
 C -3.09753 3.52169 3.23524  
 C -3.09497 2.39584 4.11842  
 C -1.85053 1.74420 4.40274  
 C -1.84735 0.37381 4.70708  
 C -0.61092 -0.33765 4.72211  
 C 0.60651 0.37104 4.72373  
 C 1.84279 -0.34057 4.70527  
 C 3.08408 0.37536 4.73045  
 C 4.30211 -0.33009 4.78682  
 C 5.49798 0.43913 4.85021  
 C 5.49496 1.77501 4.55184  
 C -5.51192 3.56970 3.35453  
 C -5.50908 2.49328 4.20008  
 C -4.30989 1.77665 4.47211  
 C -4.30663 0.36245 4.78779  
 C -3.08841 -0.34254 4.72936  
 C -5.50227 -0.40725 4.84989  
 C -5.49900 -1.74259 4.54918  
 C 0.19052 -1.47453 -0.00067  
 H 0.01560 -0.39832 -0.00031  
 H 6.43716 5.00839 -1.04693  
 H 6.43951 3.95028 -3.21240  
 H 6.44223 2.30338 -4.50569  
 H 6.44774 -0.04840 -5.03239  
 H 6.45126 -2.09057 -4.57726  
 H 6.45678 -3.98714 -3.08974  
 H 6.45957 -4.91208 -1.20616  
 H 6.45957 -4.91279 1.20338  
 H 6.45678 -3.98895 3.08751  
 H 6.45125 -2.09323 4.57611  
 H 6.44774 -0.05130 5.03238  
 H 6.44224 2.30077 4.50698  
 H 6.43952 3.94839 3.21461  
 H 6.43716 5.00776 1.04976  
 H -6.45205 0.08547 -5.03353  
 H -6.44608 -2.26610 -4.50561  
 H -6.44364 -3.91340 -3.21349  
 H -6.44178 -4.97608 -1.05009  
 H -6.44178 -4.97670 1.04727  
 H -6.44364 -3.91526 3.21128  
 H -6.44608 -2.26868 4.50433  
 H -6.45206 0.08259 5.03356  
 H -6.45646 2.12498 4.57760  
 H -6.46162 4.02069 3.08915

H -6.46340 4.94656 1.20609  
 H -6.46340 4.94727 -1.20326  
 H -6.46163 4.02246 -3.08684  
 H -6.45647 2.12760 -4.57638  
 H -0.76708 -2.00107 -0.00060  
 H 0.75777 -1.75224 -0.89254  
 H 0.75821 -1.75277 0.89075

#### Methane-graphene, gas

C 3.65226 5.67021 -0.00646  
 C 2.90568 4.48363 -0.02022  
 C 3.59519 3.24545 -0.02899  
 C 5.01948 3.23405 -0.02223  
 C 5.74317 4.45661 -0.00738  
 C 5.03555 5.65841 -0.00020  
 C 5.72220 2.00168 -0.03017  
 C 7.16211 1.99790 -0.02260  
 C 7.85983 3.26087 -0.00710  
 C 7.18335 4.42925 0.00001  
 C 2.87586 2.01074 -0.04462  
 C 3.57806 0.78973 -0.05319  
 C 5.01032 0.78505 -0.04525  
 C 5.71703 -0.44633 -0.05298  
 C 7.15401 -0.43975 -0.04507  
 C 7.83944 0.80172 -0.02998  
 C 2.87033 -0.45013 -0.06971  
 C 3.57761 -1.66798 -0.07664  
 C 5.01548 -1.67056 -0.06795  
 C 5.73387 -2.89335 -0.07448  
 C 7.16545 -2.87536 -0.06673  
 C 7.84178 -1.64892 -0.05236  
 C 5.04606 -4.14253 -0.08865  
 C 3.58124 -4.13724 -0.09599  
 C 2.87056 -2.90631 -0.09098  
 C 1.44268 -2.90244 -0.10023  
 C 0.72820 -1.66486 -0.10073  
 C 1.43717 -0.44620 -0.08073  
 C 0.73243 0.79513 -0.06937  
 C 1.44258 2.01479 -0.05198  
 C 0.73605 3.25521 -0.04079  
 C 1.44860 4.48427 -0.02530  
 C 5.79123 -5.31413 -0.09502  
 C 7.19713 -5.29381 -0.08776  
 C 7.87595 -4.10326 -0.07388  
 C 0.73423 -4.13107 -0.10889  
 C 1.46543 -5.32011 -0.11427  
 C 2.84720 -5.32210 -0.10866  
 C -0.69946 0.79824 -0.07719  
 C -1.40939 -0.43980 -0.09664  
 C -0.70618 -1.66161 -0.11419  
 C -1.42581 -2.89606 -0.11391  
 C -0.72308 -4.12775 -0.11127  
 C -0.69207 3.25836 -0.04490  
 C -1.40408 2.02108 -0.06093  
 C -2.84241 -0.43726 -0.08879  
 C -3.55519 -1.65223 -0.09311  
 C -2.85355 -2.89380 -0.10638  
 C -3.56986 -4.12159 -0.10614  
 C -2.84115 -5.30967 -0.10432  
 C -1.45936 -5.31362 -0.10487  
 C -3.54488 0.80564 -0.07212  
 C -2.83735 2.02348 -0.06111  
 C -4.97714 0.80722 -0.06766  
 C -5.68929 -0.42111 -0.07550  
 C -4.99318 -1.64844 -0.08722  
 C -5.71695 -2.86808 -0.09419  
 C -5.03467 -4.12034 -0.10542  
 C -1.39916 4.49060 -0.03271  
 C -0.66255 5.67713 -0.01796  
 C 0.71725 5.67406 -0.01444  
 C -2.85623 4.49642 -0.03484  
 C -3.55121 3.26133 -0.04711  
 C -4.97554 3.25624 -0.04545  
 C -5.68370 2.02694 -0.05502  
 C -7.12363 2.02951 -0.05149

C -7.80621 0.83633 -0.05967  
 C -7.12624 -0.40816 -0.07148  
 C -7.81934 -1.61431 -0.07958  
 C -7.14844 -2.84373 -0.09108  
 C -7.86438 -4.06849 -0.10037  
 C -7.19083 -5.26204 -0.11315  
 C -5.78503 -5.28861 -0.11608  
 C -5.69383 4.48196 -0.03311  
 C -7.13414 4.46095 -0.03051  
 C -7.81577 3.29559 -0.03909  
 C -4.98090 5.68063 -0.02327  
 C -3.59756 5.68628 -0.02395  
 C -0.73234 -1.69008 3.14853  
 H -1.75664 -1.69071 2.77115  
 H -7.65888 5.41213 -0.02086  
 H 7.71222 5.37810 0.01187  
 H -8.90636 -1.60412 -0.07699  
 H -8.89338 0.83691 -0.05686  
 H -8.90180 3.28353 -0.03666  
 H -8.94989 -4.03870 -0.09790  
 H -7.73844 -6.19877 -0.12160  
 H -5.29676 -6.25517 -0.12863  
 H -3.35151 -6.26471 -0.09857  
 H -0.95724 -6.27242 -0.09775  
 H 0.95915 -6.27665 -0.12501  
 H 3.35337 -6.27939 -0.11398  
 H 5.29872 -6.27853 -0.10635  
 H 7.74059 -6.23298 -0.09335  
 H 8.96157 -4.07828 -0.06810  
 H 8.92883 -1.64354 -0.04658  
 H 8.92658 0.79751 -0.02415  
 H 8.94579 3.24401 -0.00131  
 H -5.52576 6.62037 -0.01429  
 H -3.09277 6.64391 -0.01526  
 H -1.16667 6.63502 -0.00804  
 H 1.22560 6.62966 -0.00178  
 H 3.15172 6.63010 -0.00032  
 H 5.58453 6.59573 0.01077  
 H -0.74360 -1.69997 4.23887  
 H -0.21092 -2.57526 2.77943  
 H -0.21773 -0.79449 2.79560

#### Methane-convex surface of SWCNT, gas

C -4.00415 -1.96840 4.68707  
 C -4.21297 -0.54558 4.86449  
 C -3.11267 0.32339 4.72884  
 C -1.77840 -0.19894 4.77054  
 C -1.57606 -1.57743 4.59851  
 C -2.70788 -2.43085 4.38553  
 C -5.51009 0.04031 4.85678  
 C -5.70282 1.32170 4.41565  
 C -4.61213 2.10955 3.95134  
 C -3.31402 1.66318 4.26828  
 C -2.17429 2.43349 3.86592  
 C -2.32753 3.41850 2.87723  
 C -3.61975 3.63026 2.29423  
 C -4.77029 3.12658 2.93155  
 C -0.86213 2.02325 4.24794  
 C -0.66121 0.68669 4.70707  
 C 0.25311 2.79592 3.86684  
 C 0.09706 3.79815 2.86215  
 C -1.16847 3.99096 2.27356  
 C -1.24816 4.45545 0.92632  
 C -2.48265 4.32830 0.22360  
 C -3.69916 4.09616 0.94362  
 C -4.92744 4.05634 0.25555  
 C -6.10271 3.85903 1.03389  
 C -6.02668 3.40900 2.32458  
 C -2.46971 4.17478 -1.17097  
 C -3.67358 3.78751 -1.84433  
 C -4.91434 3.89696 -1.18538  
 C -1.22216 4.14516 -1.86154  
 C -0.04653 4.55834 -1.20366  
 C -0.06015 4.71646 0.21551

|   |          |          |          |                       |          |          |          |   |          |          |          |
|---|----------|----------|----------|-----------------------|----------|----------|----------|---|----------|----------|----------|
| C | 1.18088  | 4.80188  | 0.91436  | C                     | -0.02836 | -3.97002 | -2.84791 | C | -5.62670 | 1.43340  | -4.59258 |
| C | 1.25978  | 4.34166  | 2.23876  | C                     | 1.23739  | -4.16431 | -2.25966 | C | -1.89267 | -0.53894 | -4.68872 |
| C | 2.54713  | 4.16492  | 2.84384  | C                     | 2.39623  | -3.59141 | -2.86333 | C | -1.84010 | -1.90006 | -4.34628 |
| C | 2.70389  | 3.15957  | 3.85051  | C                     | 3.68869  | -3.80366 | -2.28096 | C | -3.05965 | -2.58883 | -4.03824 |
| C | 1.56775  | 2.36653  | 4.21773  | C                     | 4.83866  | -3.29858 | -2.91860 | C | -4.29716 | -2.03063 | -4.41388 |
| C | 1.76547  | 1.05207  | 4.66977  | C                     | 6.09567  | -3.57860 | -2.31219 | C | -3.01884 | -3.67820 | -3.11190 |
| C | 0.64816  | 0.17003  | 4.76934  | C                     | 6.17225  | -4.02611 | -1.02084 | C | -4.21765 | -4.18939 | -2.57642 |
| C | 0.85382  | -1.23165 | 4.59503  | C                     | -0.18465 | -2.96766 | -3.85243 | C | -5.42910 | -3.82478 | -3.22843 |
| C | -0.25653 | -2.06764 | 4.36395  | C                     | 0.93060  | -2.19521 | -4.23358 | C | -5.46778 | -2.78341 | -4.11583 |
| C | -1.12067 | 3.39901  | -3.07358 | C                     | 2.24267  | -2.60580 | -3.85166 | C | -1.76039 | -4.04011 | -2.52793 |
| C | -2.27066 | 2.70875  | -3.56027 | C                     | 3.38212  | -1.83552 | -4.25477 | C | -0.54143 | -3.58919 | -3.11648 |
| C | -3.57248 | 3.03937  | -3.05970 | C                     | 4.68021  | -2.28193 | -3.93858 | C | -0.58185 | -2.50194 | -4.04142 |
| C | -4.71300 | 2.40895  | -3.59391 | C                     | -4.70340 | -5.58340 | 1.23739  | C | 0.61316  | -1.82417 | -4.35958 |
| C | -5.97903 | 2.81262  | -3.08329 | C                     | -4.69043 | -5.73493 | -0.12296 | C | 0.56033  | -0.43890 | -4.70493 |
| C | -6.07627 | 3.53066  | -1.92190 | C                     | -3.53346 | -5.41187 | -0.88638 | C | -0.68545 | 0.22149  | -4.72427 |
| C | 2.39004  | 5.08482  | 0.19878  | C                     | -3.61515 | -4.93608 | -2.25263 | C | -0.73958 | 1.62207  | -4.45150 |
| C | 2.40395  | 4.92597  | -1.22373 | C                     | -2.47871 | -4.33687 | -2.83043 | C | -1.99824 | 2.22279  | -4.15111 |
| C | 1.20740  | 4.48961  | -1.88155 | C                     | -2.63554 | -3.33138 | -3.83686 | C | -1.73993 | -4.60167 | -1.24129 |
| C | 1.30783  | 3.75226  | -3.07184 | C                     | -1.49933 | -2.53831 | -4.20375 | C | -2.97695 | -4.80813 | -0.54611 |
| C | 0.15450  | 3.08612  | -3.58396 | C                     | -1.69709 | -1.22407 | -4.65645 | C | -4.19601 | -4.77492 | -1.25133 |
| C | 0.32533  | 1.89566  | -4.35214 | C                     | -0.57963 | -0.34220 | -4.75643 | C | 0.69091  | -3.95879 | -2.54262 |
| C | -0.78512 | 1.05960  | -4.58313 | C                     | 0.72971  | -0.85889 | -4.69350 | C | 0.71172  | -4.53209 | -1.23684 |
| C | -2.10265 | 1.53813  | -4.31587 | C                     | 1.84688  | 0.02668  | -4.75738 | C | -0.50041 | -4.71201 | -0.54289 |
| C | -3.23723 | 0.69945  | -4.56938 | C                     | 3.18095  | -0.49578 | -4.71559 | C | -0.49948 | -4.68170 | 0.88303  |
| C | -4.53970 | 1.19991  | -4.37337 | C                     | 4.28128  | 0.37305  | -4.85176 | C | -1.74050 | -4.52215 | 1.56730  |
| C | 3.60194  | 5.23973  | 0.89969  | C                     | 5.57826  | -0.21314 | -4.84502 | C | -2.97656 | -4.76416 | 0.88413  |
| C | 3.68361  | 4.76398  | 2.26598  | C                     | 5.77084  | -1.49454 | -4.40394 | C | -4.19631 | -4.67952 | 1.58400  |
| C | 1.64478  | 1.40528  | -4.58600 | C                     | -4.85752 | -4.75735 | -2.92413 | C | -5.38449 | -4.97641 | 0.85893  |
| C | 2.77663  | 2.25857  | -4.37260 | C                     | -5.00747 | -3.79559 | -3.88657 | C | -5.38463 | -5.02411 | -0.50921 |
| C | 2.60513  | 3.45243  | -3.60267 | C                     | -3.92609 | -2.94305 | -4.24692 | C | 1.90969  | -3.46856 | -3.09985 |
| C | 3.73286  | 4.16350  | -3.14732 | C                     | -4.13049 | -1.58661 | -4.71402 | C | 1.87141  | -2.40070 | -4.01062 |
| C | 3.62900  | 4.92510  | -1.91925 | C                     | -3.03097 | -0.70619 | -4.74178 | C | 0.71207  | -4.47654 | 1.56959  |
| C | 4.77231  | 5.41065  | -1.22393 | C                     | -5.42706 | -1.01363 | -4.84387 | C | 1.94912  | -4.59439 | 0.87062  |
| C | 4.75913  | 5.56234  | 0.13636  | C                     | -5.62426 | 0.33092  | -4.68053 | C | 1.94935  | -4.62052 | -0.53273 |
| C | 3.99438  | 2.77118  | 4.26060  | C                     | -2.98402 | 7.47496  | -0.56564 | C | 3.18691  | -4.46085 | -1.23739 |
| C | 5.07584  | 3.62356  | 3.90009  | H                     | -2.92152 | 7.33012  | 0.51372  | C | 3.16744  | -3.86527 | -2.53792 |
| C | 4.92596  | 4.58519  | 2.93750  | H                     | 7.12998  | -3.88793 | 1.51963  | C | 4.37057  | -3.43726 | -3.13324 |
| C | 4.19867  | 1.41476  | 4.72785  | H                     | 6.95852  | -2.62867 | 3.56694  | C | 4.33069  | -2.32958 | -4.06547 |
| C | 3.09925  | 0.53422  | 4.75490  | H                     | 6.70752  | -0.88346 | 4.69626  | C | 3.09014  | -1.72568 | -4.34975 |
| C | 3.30553  | -0.87133 | 4.58183  | H                     | 6.35978  | 1.48442  | 4.98274  | C | 3.03700  | -0.34065 | -4.70651 |
| C | 2.17128  | -1.71017 | 4.32746  | H                     | 6.06372  | 3.44754  | 4.31103  | C | 1.76738  | 0.32396  | -4.70463 |
| C | 4.07279  | 1.79588  | -4.67401 | H                     | 5.79975  | 5.14066  | 2.61549  | C | 1.71352  | 1.70140  | -4.43895 |
| C | 5.15028  | 2.70529  | -4.47923 | H                     | 5.68137  | 5.82952  | 0.64027  | C | 0.45404  | 2.31562  | -4.16978 |
| C | 4.98608  | 3.84745  | -3.74305 | H                     | 5.70474  | 5.56520  | -1.75514 | C | 3.18834  | -4.39858 | 1.56372  |
| C | 4.60798  | -1.37146 | 4.38618  | H                     | 5.85642  | 4.45717  | -3.52764 | C | 4.41065  | -4.59136 | 0.89064  |
| C | 5.69237  | -0.50266 | 4.69471  | H                     | 6.14519  | 2.44671  | -4.82413 | C | 4.40999  | -4.62447 | -0.55768 |
| C | 5.49514  | 0.84181  | 4.85847  | H                     | 6.44588  | 0.38922  | -5.09007 | C | 5.60350  | -4.48544 | -1.32070 |
| C | -0.08542 | -3.25809 | 3.59581  | H                     | 6.78475  | -1.86751 | -4.31124 | C | 5.58532  | -3.91011 | -2.56233 |
| C | 1.18988  | -3.57166 | 3.08531  | H                     | 7.01401  | -3.33568 | -2.83502 | C | 4.22502  | 0.41271  | -4.78461 |
| C | 2.33963  | -2.88098 | 3.57190  | H                     | 7.14896  | -4.12522 | -0.56038 | C | 5.45198  | -0.30742 | -4.81630 |
| C | 3.64159  | -3.21142 | 3.07145  | H                     | -6.37776 | -0.56239 | 5.10088  | C | 5.50316  | -1.62992 | -4.46778 |
| C | 4.78165  | -2.57993 | 3.60601  | H                     | -6.71680 | 1.69427  | 4.32188  | C | 4.16917  | 1.83508  | -4.51612 |
| C | -2.53624 | -3.62473 | 3.61577  | H                     | -6.94560 | 3.16709  | 2.84692  | C | 2.93003  | 2.41372  | -4.17970 |
| C | -1.23895 | -3.92417 | 3.08460  | H                     | -7.07940 | 3.96124  | 0.57402  | C | 0.41083  | 3.46827  | -3.32945 |
| C | -1.13865 | -4.66105 | 1.89417  | H                     | -7.06059 | 3.72434  | -1.51013 | C | 1.62836  | 3.97256  | -2.78219 |
| C | 0.11515  | -4.72996 | 1.21639  | H                     | -6.88991 | 2.46143  | -3.55517 | C | 2.88668  | 3.56974  | -3.33757 |
| C | 1.29169  | -4.32022 | 1.87455  | H                     | -6.63945 | 0.71170  | -4.68114 | C | 4.08358  | 4.12417  | -2.84308 |
| C | 2.54045  | -4.35581 | 1.18499  | H                     | -6.29182 | -1.65628 | -4.96699 | C | 5.29634  | 3.71482  | -3.46564 |
| C | 3.74349  | -3.96118 | 1.85702  | H                     | -5.99536 | -3.61966 | -4.29754 | C | 5.33781  | 2.61047  | -4.27292 |
| C | 4.98407  | -4.06544 | 1.19728  | H                     | -5.73125 | -5.31295 | -2.60216 | C | -2.04063 | 3.35438  | -3.32097 |
| C | 6.14566  | -3.69709 | 1.93267  | H                     | -5.61268 | -6.00232 | -0.62674 | C | -0.82451 | 3.88464  | -2.79519 |
| C | 6.04806  | -2.98105 | 3.09519  | H                     | -5.63570 | -5.73829 | 1.76873  | C | -0.84782 | 4.55735  | -1.53656 |
| C | 0.12854  | -4.88836 | -0.20224 | H                     | -5.78730 | -4.63036 | 3.54152  | C | 0.36450  | 4.78812  | -0.85657 |
| C | 1.31751  | -4.63127 | -0.91305 | H                     | -6.07633 | -2.61975 | 4.83781  | C | 1.60556  | 4.63339  | -1.54406 |
| C | 2.55348  | -4.51138 | -0.21032 | H                     | -3.78365 | 6.84893  | -0.96650 | C | 2.84128  | 4.88870  | -0.86415 |
| C | 3.76898  | -4.27122 | -0.93076 | H                     | -3.19211 | 8.52258  | -0.78546 | C | 4.06025  | 4.80630  | -1.56548 |
| C | 4.99724  | -4.22554 | -0.24288 | H                     | -2.03595 | 7.18541  | -1.02246 | C | 0.36573  | 4.83923  | 0.56977  |
| C | -5.08143 | -2.87811 | 4.49271  | Propanamide-concave   |          |          |          | C | 1.60782  | 4.73114  | 1.26418  |
| C | -4.91708 | -4.02036 | 3.75669  | surface of SWCNT, gas |          |          |          | C | 2.84226  | 4.93925  | 0.56611  |
| C | -3.66391 | -4.33610 | 3.16075  | C                     | -5.57527 | 0.09116  | -4.85736 | C | 4.06279  | 4.90249  | 1.26838  |
| C | -3.56016 | -5.09754 | 1.93259  | C                     | -4.35008 | -0.62776 | -4.77250 | C | 5.24934  | 5.15787  | 0.52447  |
| C | -2.33528 | -5.09773 | 1.23681  | C                     | -3.16145 | 0.12725  | -4.73224 | C | 5.24842  | 5.11141  | -0.84341 |
| C | -2.32161 | -5.25645 | -0.18552 | C                     | -3.21535 | 1.53073  | -4.45759 | C | -3.30075 | 3.79024  | -2.79502 |
| C | -1.11254 | -4.97322 | -0.90094 | C                     | -4.45655 | 2.15557  | -4.22508 | C | -3.32391 | 4.46218  | -1.53178 |
| C | -1.19135 | -4.51350 | -2.22532 |                       |          |          |          | C | -2.08709 | 4.67632  | -0.83964 |

C -2.08588 4.72450 0.56341  
 C -0.84547 4.65321 1.26540  
 C -0.81969 4.06787 2.56678  
 C 0.41641 3.68677 3.12486  
 C 1.63319 4.15312 2.54286  
 C 2.89287 3.78562 3.11975  
 C 4.08931 4.30650 2.58846  
 C 0.46115 2.59191 4.03873  
 C 1.72046 1.99331 4.34005  
 C 2.93703 2.68592 4.03374  
 C 4.17671 2.12562 4.39903  
 C 5.34545 2.88334 4.10551  
 C 5.30366 3.93618 3.23194  
 C -3.32193 4.55820 1.27047  
 C -3.29584 3.97287 2.57588  
 C -2.03499 3.57327 3.12750  
 C -1.99089 2.49763 4.02826  
 C -0.73178 1.91618 4.36306  
 C -0.67749 0.53431 4.71453  
 C 0.56648 -0.12604 4.72458  
 C 1.77339 0.63291 4.68084  
 C 3.04173 -0.03264 4.71877  
 C 4.23146 0.72174 4.75219  
 C 0.61772 -1.52608 4.45820  
 C 1.87310 -2.13094 4.15715  
 C 3.09205 -1.43769 4.45264  
 C 4.33245 -2.06490 4.22312  
 C 5.50547 -1.34070 4.57702  
 C 5.45702 0.00339 4.83242  
 C -3.20781 1.82619 4.37907  
 C -3.15293 0.44190 4.73803  
 C -1.88450 -0.22527 4.72903  
 C -1.83379 -1.60341 4.46690  
 C -0.57754 -2.22054 4.19077  
 C -0.53879 -3.37796 3.35801  
 C 0.69245 -3.80838 2.82952  
 C 1.91013 -3.27390 3.34405  
 C 3.16816 -3.71687 2.82160  
 C 4.37099 -3.24213 3.38062  
 C 5.60618 -4.40461 1.64061  
 C 5.58675 -3.75184 2.84295  
 C -3.05401 -2.31137 4.21323  
 C -3.01654 -3.46279 3.36488  
 C -1.75992 -3.86994 2.80887  
 C -4.21679 -4.00792 2.86739  
 C -5.42751 -3.59823 3.49341  
 C -5.46296 -2.49953 4.30874  
 C -4.29086 -1.73018 4.55445  
 C -4.34230 -0.30799 4.82613  
 C -5.56722 0.41519 4.87021  
 C -5.61954 1.73873 4.52482  
 C -4.44947 2.43554 4.11107  
 C -4.49507 3.54224 3.17679  
 C -5.71292 4.00639 2.60447  
 C -5.73790 4.56629 1.35552  
 C -4.54633 4.70143 0.58888  
 C -4.54726 4.64996 -0.85940  
 C -5.73998 4.46231 -1.61297  
 C -5.71789 3.82149 -2.82264  
 C -4.50073 3.32116 -3.36520  
 O 0.63551 -1.66293 0.88193  
 C 0.80967 -1.17009 -0.22153  
 N -0.19528 -1.05494 -1.13013  
 C 2.15500 -0.62135 -0.67795  
 C 3.27555 -1.00696 0.27728  
 H 6.19477 5.28547 1.03961  
 H 6.19303 5.20377 -1.36783  
 H 6.22626 4.21497 -3.21926  
 H 6.29888 2.27014 -4.64168  
 H 6.38143 0.21497 -5.01299  
 H 6.47139 -2.11301 -4.39731  
 H 6.52802 -3.72502 -3.06482  
 H 6.56053 -4.73721 -0.87736  
 H 6.56336 -4.68000 1.21188  
 H 6.52920 -3.53110 3.33175

H 6.47276 -1.82984 4.54485  
 H 6.38748 0.53542 4.99579  
 H 6.30740 2.56393 4.49083  
 H 6.23383 4.41832 2.95253  
 H -6.59454 1.92144 -4.56288  
 H -6.50424 -0.44046 -5.03034  
 H -6.42840 -2.46707 -4.50694  
 H -6.36063 -4.30203 -2.94543  
 H -6.33009 -5.14861 -1.02503  
 H -6.33024 -5.06379 1.38207  
 H -6.36004 -4.09237 3.24420  
 H -6.42236 -2.15697 4.68004  
 H -6.49561 -0.10549 5.07689  
 H -6.58726 2.22473 4.46746  
 H -6.65394 3.82060 3.11024  
 H -6.69754 4.80555 0.91075  
 H -6.69858 4.73081 -1.18319  
 H -6.65950 3.60267 -3.31368  
 H 4.21450 -0.53164 -0.01514  
 H 3.02730 -0.71271 1.30100  
 H 3.42309 -2.08981 0.27497  
 H 2.05953 0.46977 -0.75643  
 H 2.35923 -0.98396 -1.69398  
 H -0.05409 -0.64754 -2.04169  
 H -1.11035 -1.39770 -0.87934

#### Propanamide-graphene, gas

C 3.70334 5.62327 -0.17872  
 C 2.96124 4.43391 -0.19615  
 C 3.65543 3.19795 -0.18984  
 C 5.07970 3.19122 -0.16247  
 C 5.79852 4.41663 -0.14263  
 C 5.08646 5.61582 -0.15194  
 C 7.22635 1.96217 -0.13067  
 C 7.91896 3.22795 -0.10949  
 C 7.23851 4.39408 -0.11511  
 C 2.94079 1.96024 -0.21048  
 C 3.64759 0.74142 -0.20423  
 C 5.07962 0.74183 -0.17600  
 C 5.79050 -0.48743 -0.17072  
 C 7.22749 -0.47591 -0.14734  
 C 7.90792 0.76835 -0.12722  
 C 2.94429 -0.50114 -0.21924  
 C 3.65543 -1.71672 -0.20960  
 C 5.09311 -1.71430 -0.18683  
 C 5.81568 -2.93486 -0.18196  
 C 7.24721 -2.91163 -0.16339  
 C 7.91923 -1.68285 -0.14547  
 C 5.13212 -4.18659 -0.19619  
 C 3.66725 -4.18599 -0.20705  
 C 2.95242 -2.95758 -0.21538  
 C 1.52447 -2.95929 -0.22638  
 C 0.80544 -1.72405 -0.24629  
 C 1.51101 -0.50205 -0.24904  
 C 0.80081 0.73692 -0.26249  
 C 1.50743 1.95933 -0.24544  
 C 0.79637 3.19777 -0.25508  
 C 1.50418 4.42922 -0.22344  
 C 5.88106 -5.35581 -0.19711  
 C 7.28676 -5.33015 -0.18115  
 C 7.96158 -4.13739 -0.16342  
 C 0.81965 -4.18991 -0.21667  
 C 1.55496 -5.37647 -0.21193  
 C 2.93676 -5.37319 -0.20805  
 C -0.63097 0.73512 -0.29590  
 C -1.33667 -0.50484 -0.28008  
 C -0.62924 -1.72502 -0.26220  
 C -1.34448 -2.96186 -0.23927  
 C -0.63756 -4.19076 -0.21231  
 C -0.63258 3.19501 -0.29228  
 C -1.34081 1.95518 -0.30893  
 C -2.76954 -0.50595 -0.28439  
 C -3.47742 -1.72347 -0.26474  
 C -2.77219 -2.96340 -0.24279

C -3.48444 -4.19319 -0.21840  
 C -2.75218 -5.37874 -0.18216  
 C -1.37037 -5.37832 -0.17864  
 C -3.47522 0.73342 -0.30041  
 C -2.77261 1.95294 -0.31436  
 C -4.90619 0.73012 -0.30467  
 C -5.61449 -0.49977 -0.28986  
 C -4.91518 -1.72453 -0.26853  
 C -5.63486 -2.94619 -0.25336  
 C -4.94912 -4.19606 -0.23023  
 C -1.34423 4.42550 -0.28943  
 C -0.61179 5.61480 -0.24374  
 C 0.76752 5.61639 -0.21351  
 C -2.80054 4.42535 -0.32527  
 C -3.48985 3.18756 -0.32515  
 C -4.91378 3.17833 -0.33714  
 C -5.61735 1.94690 -0.32547  
 C -7.05707 1.94529 -0.33451  
 C -7.73586 0.74998 -0.32066  
 C -7.05107 -0.49152 -0.29752  
 C -7.74072 -1.69956 -0.28401  
 C -7.06619 -2.92688 -0.26229  
 C -7.77886 -4.15335 -0.25010  
 C -7.10205 -5.34502 -0.23130  
 C -5.69616 -5.36646 -0.22189  
 C -5.63626 4.40125 -0.35978  
 C -7.07648 4.37599 -0.37114  
 C -7.75405 3.20833 -0.35853  
 C -4.92805 5.60299 -0.37220  
 C -3.54506 5.61300 -0.35489  
 C -0.42879 -0.46110 3.06157  
 C -1.09936 0.88173 2.81429  
 C -1.44164 -1.59112 3.16706  
 H -7.60410 5.32540 -0.38910  
 H 7.76410 5.34471 -0.09928  
 H -8.82782 -1.69264 -0.29012  
 H -8.82304 0.74668 -0.32641  
 H -8.84000 3.19225 -0.36550  
 H -8.86445 -4.12657 -0.25678  
 H -7.64659 -6.28348 -0.22349  
 H -5.20472 -6.33146 -0.20867  
 H -3.25953 -6.33497 -0.15328  
 H -0.86528 -6.33505 -0.14537  
 H 1.05199 -6.33482 -0.21384  
 H 3.44640 -6.32866 -0.20310  
 H 5.39205 -6.32194 -0.21140  
 H 7.83364 -6.26739 -0.18261  
 H 9.04703 -4.10893 -0.14995  
 H 9.00612 -1.67383 -0.12999  
 H 8.99491 0.76816 -0.10888  
 H 9.00481 3.21512 -0.08926  
 H -5.47609 6.54057 -0.39478  
 H -3.04297 6.57213 -0.36843  
 H -1.12019 6.57026 -0.22594  
 H 1.27196 6.57349 -0.17614  
 H 3.19962 6.58143 -0.18999  
 H 5.63209 6.55509 -0.13919  
 H -2.06174 -1.47194 4.05835  
 H -2.11245 -1.58125 2.30521  
 H -0.93924 -2.56047 3.21375  
 H 0.17939 -0.38284 3.97036  
 H 0.27545 -0.64032 2.23838  
 N -0.25171 1.95740 2.82486  
 O -2.29866 1.00263 2.64281  
 H 0.73904 1.81576 2.69955  
 H -0.63449 2.82803 2.48447

#### Propanamide-convex surface of SWCNT, gas

C -0.06634 -5.49862 -4.86379  
 C 0.78003 -4.38612 -4.59593  
 C 0.21378 -3.10158 -4.71572  
 C -1.20798 -2.95072 -4.76843  
 C -2.03848 -4.08685 -4.70048  
 C -1.42662 -5.35432 -4.91403



|   |          |          |          |   |          |          |          |                        |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|------------------------|----------|----------|----------|
| C | 1.02451  | -1.93921 | -4.50005 | C | -5.14758 | -0.08214 | 0.17428  | H                      | -1.04962 | 6.54277  | 4.92709  |
| C | 2.25847  | -2.07561 | -3.84444 | C | -4.88233 | -0.12292 | 1.57629  | H                      | -2.88788 | 6.74534  | 3.94608  |
| C | 2.67820  | -3.37400 | -3.40418 | C | -4.47257 | 1.05388  | 2.23360  | H                      | -4.31091 | 6.91252  | 2.00857  |
| C | 2.05314  | -4.52677 | -3.91825 | C | -4.61119 | 2.31621  | 1.58259  | H                      | -2.04150 | -6.24248 | -5.01004 |
| C | 3.52029  | -3.47282 | -2.25144 | C | -4.21667 | 3.51864  | 2.25581  | H                      | 0.35437  | -6.49620 | -4.92429 |
| C | 3.72421  | -4.72218 | -1.63311 | C | -4.42101 | 4.76914  | 1.63961  | H                      | 2.19012  | -6.70002 | -3.93776 |
| C | 3.34883  | -5.88106 | -2.36962 | C | -3.62959 | 0.95505  | 3.38102  | H                      | 3.61115  | -6.86568 | -1.99902 |
| C | 2.54181  | -5.78668 | -3.47109 | C | -2.95032 | 2.12130  | 3.84422  | H                      | 4.01095  | -6.92308 | 0.05927  |
| C | 3.91080  | -2.26937 | -1.57766 | C | -3.37199 | 3.41958  | 3.40675  | H                      | 3.39566  | -6.87680 | 2.38744  |
| C | 3.77677  | -1.00767 | -2.23183 | C | -2.74738 | 4.57236  | 3.92158  | H                      | 2.03716  | -6.74590 | 3.98332  |
| C | 2.93830  | -0.90913 | -3.38272 | C | -3.23834 | 5.83246  | 3.47763  | H                      | -0.16188 | -6.52238 | 4.94443  |
| C | 2.53495  | 0.36378  | -3.83341 | C | -4.04642 | 5.92759  | 2.37718  | H                      | -2.24543 | -6.30285 | 4.85536  |
| C | 1.27988  | 0.50214  | -4.49912 | C | -5.41350 | -2.54561 | 0.15216  | H                      | -4.36137 | -6.07021 | 3.72571  |
| C | 0.47297  | -0.63686 | -4.69142 | C | -5.14703 | -2.58662 | 1.55772  | H                      | -5.60881 | -5.92321 | 2.04726  |
| C | -0.94532 | -0.48670 | -4.74346 | C | -4.71127 | -1.38847 | 2.21286  | H                      | -6.05719 | -5.85391 | -0.32101 |
| C | -1.77022 | -1.64253 | -4.60320 | C | -3.88115 | -1.48587 | 3.34079  | H                      | -5.51340 | -5.89607 | -2.34208 |
| C | 4.16502  | -2.30721 | -0.19736 | C | -3.22490 | -0.31756 | 3.83075  | H                      | -3.95026 | -6.04714 | -4.17047 |
| C | 4.03801  | -3.54927 | 0.50625  | C | -1.97026 | -0.45535 | 4.49763  | H                      | 7.50304  | -3.40653 | 0.09250  |
| C | 3.99430  | -4.76188 | -0.20952 | C | -1.16421 | 0.68378  | 4.69194  | H                      | 6.74889  | -2.24369 | 1.20222  |
| C | 4.18191  | 0.16977  | -1.57193 | C | -1.71646 | 1.98567  | 4.50028  | H                      | 8.50138  | -2.30644 | 1.07043  |
| C | 4.43389  | 0.13118  | -0.16794 | C | -0.90673 | 3.14835  | 4.71748  | H                      | 8.38339  | -1.46155 | -1.28699 |
| C | 4.28520  | -1.08376 | 0.52728  | C | -1.47378 | 4.43252  | 4.59812  | H                      | 6.62900  | -1.49359 | -1.23265 |
| C | 3.93398  | -1.05684 | 1.90991  | C | 0.25391  | 0.53422  | 4.74814  | H                      | 7.28488  | 0.82416  | -1.97485 |
| C | 3.46030  | -2.25377 | 2.52425  | C | 1.07860  | 1.69047  | 4.60894  | H                      | 7.34015  | 1.98176  | -0.69858 |
| C | 3.67795  | -3.52131 | 1.89120  | C | 0.51511  | 2.99844  | 4.77186  | Propanoic acid-concave |          |          |          |
| C | 3.27291  | -4.70734 | 2.53448  | C | 1.34493  | 4.13511  | 4.70383  | surface of SWCNT, gas  |          |          |          |
| C | 3.55717  | -5.93559 | 1.87374  | C | 0.73209  | 5.40228  | 4.91678  | C                      | 4.37849  | -0.06929 | 4.77560  |
| C | 3.90589  | -5.96209 | 0.55042  | C | -0.62819 | 5.54560  | 4.86625  | C                      | 4.35532  | -1.50050 | 4.55140  |
| C | 4.01689  | 1.43509  | -2.21162 | C | -3.48776 | -2.78151 | 3.81118  | C                      | 3.12755  | -2.12019 | 4.24696  |
| C | 3.19107  | 1.53232  | -3.34279 | C | -2.23002 | -2.91966 | 4.48009  | C                      | 1.89537  | -1.43216 | 4.49742  |
| C | 3.73667  | 0.18440  | 2.54574  | C | -1.40926 | -1.75780 | 4.65560  | C                      | 1.91853  | -0.04473 | 4.71126  |
| C | 4.17900  | 1.38387  | 1.91317  | C | -0.01444 | -1.90516 | 4.71154  | C                      | 3.17152  | 0.65072  | 4.67894  |
| C | 4.52671  | 1.35630  | 0.55531  | C | 0.81698  | -0.75007 | 4.60868  | C                      | 5.54069  | -2.25205 | 4.31496  |
| C | 4.71275  | 2.59092  | -0.14664 | C | 2.11956  | -0.88272 | 4.03969  | C                      | 5.51943  | -3.37648 | 3.53512  |
| C | 4.45122  | 2.63283  | -1.55443 | C | 2.81295  | 0.27343  | 3.62965  | C                      | 4.31062  | -3.83022 | 2.93557  |
| C | 4.35323  | 3.87271  | -2.21615 | C | 2.35935  | 1.56008  | 4.04840  | C                      | 3.10493  | -3.29751 | 3.43343  |
| C | 3.49657  | 3.97414  | -3.38054 | C | 3.07289  | 2.73776  | 3.65001  | C                      | 1.85038  | -3.74391 | 2.90158  |
| C | 2.79867  | 2.82851  | -3.81229 | C | 2.66553  | 4.00072  | 4.12271  | C                      | 1.83223  | -4.42318 | 1.67233  |
| C | 1.54034  | 2.96693  | -4.48020 | C | 4.32876  | 5.03971  | 2.68583  | C                      | 3.06753  | -4.66026 | 0.98343  |
| C | 0.71911  | 1.80506  | -4.65501 | C | 3.44011  | 5.12640  | 3.72351  | C                      | 4.29149  | -4.53576 | 1.67035  |
| C | -0.67585 | 1.95269  | -4.70613 | C | 0.55672  | -3.21441 | 4.59172  | C                      | 0.62655  | -3.26412 | 3.45674  |
| C | -1.50734 | 0.79771  | -4.60118 | C | 1.86256  | -3.34733 | 4.02110  | C                      | 0.64961  | -2.08635 | 4.26236  |
| C | 3.99993  | 2.64768  | 2.56392  | C | 2.55162  | -2.16649 | 3.59096  | C                      | 0.58951  | -4.62037 | 0.99864  |
| C | 4.50642  | 3.82147  | 1.97221  | C | 2.33449  | -4.61723 | 3.63494  | C                      | -0.62068 | -4.40747 | 1.68783  |
| C | 4.87912  | 3.79086  | 0.57248  | C | 1.63189  | -5.75116 | 4.13111  | C                      | -0.60172 | -3.71690 | 2.93651  |
| C | 5.10469  | 4.97635  | -0.18385 | C | 0.38338  | -5.62411 | 4.67729  | C                      | -1.82635 | -3.20300 | 3.45875  |
| C | 4.84928  | 5.01680  | -1.52844 | C | -0.25271 | -4.35375 | 4.76655  | C                      | -1.80397 | -2.04487 | 4.25245  |
| C | 1.00203  | 4.24935  | -4.70533 | C | -1.69228 | -4.20186 | 4.70815  | C                      | -0.55686 | -1.40817 | 4.52406  |
| C | 1.87944  | 5.35964  | -4.55321 | C | -2.56985 | -5.31210 | 4.55738  | C                      | -0.53402 | 0.00133  | 4.74369  |
| C | 3.08254  | 5.22729  | -3.91341 | C | -3.77249 | -5.17993 | 3.91677  | C                      | 0.69483  | 0.68752  | 4.68892  |
| C | -0.43756 | 4.40123  | -4.76124 | C | -4.18574 | -3.92748 | 3.38161  | C                      | -1.86220 | -4.57602 | 1.00476  |
| C | -1.24654 | 3.26190  | -4.58441 | C | -5.04334 | -3.82682 | 2.21796  | C                      | -3.09811 | -4.38002 | 1.70428  |
| C | -2.80836 | 0.93045  | -4.02883 | C | -5.53364 | -4.97284 | 1.53064  | C                      | -3.08018 | -3.67789 | 2.95096  |
| C | -3.23983 | 2.21421  | -3.57958 | C | -5.78914 | -4.93361 | 0.18629  | C                      | -4.28694 | -3.22186 | 3.51810  |
| C | -2.55145 | 3.39480  | -4.01136 | C | -5.57221 | -3.74594 | -0.56747 | C                      | -4.26341 | -2.03001 | 4.34129  |
| C | -3.02311 | 4.66473  | -3.62536 | C | -5.19947 | -3.77445 | -1.96734 | C                      | -3.03486 | -1.37065 | 4.54335  |
| C | -2.32127 | 5.79857  | -4.12306 | C | -5.02275 | -4.99153 | -2.68356 | C                      | -3.01162 | 0.04181  | 4.77058  |
| C | -1.07364 | 5.67164  | -4.67094 | C | -4.13455 | -5.07739 | -3.72176 | C                      | -1.75831 | 0.73239  | 4.69254  |
| C | -3.04980 | -1.51186 | -4.03980 | C | -3.35874 | -3.95190 | -4.11879 | C                      | -4.32269 | -4.62176 | 1.05174  |
| C | -3.50186 | -0.22547 | -3.61885 | C | 7.52543  | -1.36030 | -0.61160 | C                      | -5.51258 | -4.44395 | 1.81178  |
| C | -4.42805 | -0.13621 | -2.53645 | C | 7.51044  | 0.05962  | -0.06520 | C                      | -5.49582 | -3.76723 | 3.00164  |
| C | -4.62737 | 1.10546  | -1.90081 | O | 7.50826  | 0.31278  | 1.12454  | C                      | -4.21703 | 0.77086  | 4.79573  |
| C | -4.14990 | 2.30204  | -2.51427 | C | 7.57341  | -2.39579 | 0.50167  | C                      | -5.42500 | 0.02773  | 4.91365  |
| C | -4.36915 | 3.56997  | -1.88287 | N | 7.52160  | 1.04163  | -1.01957 | C                      | -5.44747 | -1.32339 | 4.69356  |
| C | -3.96227 | 4.75552  | -2.52589 | H | -4.69815 | 6.97128  | -0.05087 | C                      | -1.74107 | 2.08069  | 4.30268  |
| C | -4.99338 | 1.13330  | -0.52142 | H | -4.08104 | 6.92537  | -2.37856 | C                      | -2.97711 | 2.73634  | 3.99150  |
| C | -4.87137 | 2.35619  | 0.20356  | H | -2.72658 | 6.79334  | -3.97510 | C                      | -4.19889 | 2.16315  | 4.39583  |
| C | -4.73583 | 3.59770  | -0.49966 | H | -0.52916 | 6.56995  | -4.93927 | C                      | 0.71265  | 2.05749  | 4.29065  |
| C | -4.68861 | 4.81000  | 0.21614  | H | 1.55388  | 6.35072  | -4.84833 | C                      | -0.49958 | 2.69500  | 3.96079  |
| C | -4.59538 | 6.01050  | -0.54292 | H | 3.67000  | 6.11777  | -3.71947 | C                      | -0.49221 | 3.76155  | 3.01317  |
| C | -4.24541 | 5.98431  | -1.86567 | H | 4.93099  | 5.96645  | -2.04532 | C                      | -1.72687 | 4.18234  | 2.43480  |
| C | -3.76452 | -2.68938 | -3.64321 | H | 5.38039  | 5.89489  | 0.32261  | C                      | -2.96978 | 3.80590  | 3.04131  |
| C | -4.69318 | -2.59988 | -2.55793 | H | 4.81900  | 5.94412  | 2.34329  | C                      | -4.18475 | 4.28297  | 2.51108  |
| C | -4.87475 | -1.33609 | -1.90657 | H | 3.25480  | 6.09667  | 4.17050  | C                      | -5.38117 | 3.90806  | 3.18483  |
| C | -5.23448 | -1.30865 | -0.54970 | H | 1.34648  | 6.29068  | 5.01338  |                        |          |          |          |

|   |          |          |          |                          |          |          |          |   |          |          |          |
|---|----------|----------|----------|--------------------------|----------|----------|----------|---|----------|----------|----------|
| C | -5.38799 | 2.88493  | 4.09415  | C                        | 5.46265  | -2.76060 | -4.09139 | C | 2.94598  | -0.49970 | -0.21148 |
| C | -1.73166 | 4.72363  | 1.14003  | C                        | 4.27002  | -2.04759 | -4.40018 | C | 3.65736  | -1.71522 | -0.20408 |
| C | -2.97987 | 4.88271  | 0.45322  | C                        | 4.28274  | -0.65667 | -4.80508 | C | 5.09511  | -1.71248 | -0.18748 |
| C | -4.18987 | 4.83903  | 1.17348  | C                        | 5.48806  | 0.08955  | -4.93114 | C | 5.81798  | -2.93276 | -0.18419 |
| C | 0.72729  | 4.15285  | 2.42645  | C                        | 5.50862  | 1.44082  | -4.71276 | C | 7.24947  | -2.90925 | -0.17243 |
| C | 0.72256  | 4.70372  | 1.11012  | C                        | 4.32469  | 2.14422  | -4.35349 | C | 7.92114  | -1.68022 | -0.16012 |
| C | -0.50159 | 4.84125  | 0.42582  | C                        | 4.35013  | 3.33651  | -3.53061 | C | 5.13490  | -4.18465 | -0.19313 |
| C | -0.51770 | 4.75241  | -0.99880 | C                        | 5.56117  | 3.88245  | -3.01889 | C | 3.67004  | -4.18473 | -0.19871 |
| C | -1.76309 | 4.54715  | -1.66437 | C                        | 5.58329  | 4.55630  | -1.82749 | C | 2.95488  | -2.95641 | -0.20630 |
| C | -2.99579 | 4.79077  | -0.97500 | C                        | 4.39596  | 4.73348  | -1.06305 | C | 1.52701  | -2.95836 | -0.21426 |
| C | -4.22149 | 4.65616  | -1.65606 | C                        | 4.41222  | 4.82047  | 0.38338  | C | 0.80803  | -1.72317 | -0.23363 |
| C | -5.40714 | 4.95439  | -0.92685 | C                        | 5.61643  | 4.73175  | 1.13732  | C | 1.51287  | -0.50079 | -0.23763 |
| C | -5.39193 | 5.04350  | 0.43881  | C                        | 5.62086  | 4.20502  | 2.40072  | C | 0.80326  | 0.73787  | -0.24990 |
| C | -1.78536 | 3.85041  | -2.88292 | C                        | 4.42138  | 3.73011  | 3.00190  | C | 1.50889  | 1.95954  | -0.23148 |
| C | -3.04020 | 3.39743  | -3.40719 | C                        | 4.41320  | 2.65092  | 3.96885  | C | 0.79811  | 3.19712  | -0.23415 |
| C | -4.24472 | 3.93550  | -2.91254 | C                        | 5.60421  | 1.99396  | 4.38790  | C | 1.50513  | 4.42888  | -0.20218 |
| C | 0.69122  | 4.53192  | -1.68815 | C                        | 5.58737  | 0.68198  | 4.77750  | C | 5.88437  | -5.35355 | -0.19480 |
| C | 0.66861  | 3.82528  | -2.92817 | H                        | -6.36007 | 5.00756  | -1.44158 | C | 7.29014  | -5.32774 | -0.18526 |
| C | -0.56256 | 3.36121  | -3.43245 | H                        | -6.33359 | 5.16449  | 0.96248  | C | 7.96446  | -4.13461 | -0.17329 |
| C | -0.58682 | 2.18249  | -4.23666 | H                        | -6.32535 | 4.36100  | 2.90332  | C | 0.82263  | -4.18918 | -0.20274 |
| C | -1.83281 | 1.52813  | -4.46893 | H                        | -6.33731 | 2.55850  | 4.50419  | C | 1.55819  | -5.37554 | -0.19762 |
| C | -3.06418 | 2.21553  | -4.21364 | H                        | -6.36473 | 0.54369  | 5.07563  | C | 2.94005  | -5.37220 | -0.19635 |
| C | -4.29228 | 1.59439  | -4.51351 | H                        | -6.40366 | -1.83466 | 4.68717  | C | -0.62818 | 0.73549  | -0.28505 |
| C | -5.47778 | 2.34494  | -4.27528 | H                        | -6.43810 | -3.55775 | 3.49558  | C | -1.33442 | -0.50470 | -0.27119 |
| C | -5.45518 | 3.47462  | -3.50296 | H                        | -6.46760 | -4.75152 | 1.40091  | C | -0.62665 | -1.72492 | -0.25167 |
| C | -1.85303 | 0.14175  | -4.68869 | H                        | -6.48651 | -4.90132 | -0.68406 | C | -1.34191 | -2.96196 | -0.22934 |
| C | -3.10475 | -0.55458 | -4.65632 | H                        | -6.49558 | -3.98515 | -2.91369 | C | -0.63461 | -4.19072 | -0.19891 |
| C | -4.31334 | 0.16432  | -4.74371 | H                        | -6.48797 | -2.41403 | -4.29791 | C | -0.63079 | 3.19508  | -0.27064 |
| C | 0.62015  | 1.50970  | -4.51054 | H                        | -6.46494 | -0.09536 | -4.95451 | C | -1.33889 | 1.95523  | -0.29572 |
| C | 0.59892  | 0.10068  | -4.73401 | H                        | -6.43452 | 1.96763  | -4.61870 | C | -2.76768 | -0.50652 | -0.28236 |
| C | -0.62777 | -0.58870 | -4.67550 | H                        | -6.39475 | 3.95663  | -3.25689 | C | -3.47542 | -1.72427 | -0.26397 |
| C | -0.64077 | -1.96131 | -4.28890 | H                        | 6.55991  | 2.49880  | 4.30116  | C | -2.76979 | -2.96386 | -0.23765 |
| C | -1.87954 | -2.56538 | -3.92284 | H                        | 6.53024  | 0.18880  | 4.98633  | C | -3.48177 | -4.19388 | -0.21342 |
| C | -3.11779 | -1.93148 | -4.26802 | H                        | 6.49662  | -1.87822 | 4.66426  | C | -2.74904 | -5.37892 | -0.17139 |
| C | -4.34043 | -2.56449 | -3.97039 | H                        | 6.45919  | -3.85829 | 3.28924  | C | -1.36721 | -5.37835 | -0.16384 |
| C | -5.53380 | -1.90553 | -4.37949 | H                        | 6.43068  | -4.88422 | 1.45881  | C | -3.47390 | 0.73288  | -0.30160 |
| C | -5.52079 | -0.58881 | -4.75231 | H                        | 6.41009  | -5.02617 | -0.94613 | C | -2.77123 | 1.95265  | -0.31058 |
| C | -1.88331 | -3.62357 | -3.00133 | H                        | 6.40612  | -4.22102 | -2.88621 | C | -4.90510 | 0.72915  | -0.31335 |
| C | -3.12723 | -4.03942 | -2.42202 | H                        | 6.41129  | -2.43043 | -4.49986 | C | -5.61308 | -0.50121 | -0.30169 |
| C | -4.34511 | -3.65270 | -3.01501 | H                        | 6.42794  | -0.42429 | -5.09912 | C | -4.91325 | -1.72584 | -0.27529 |
| C | 0.57287  | -2.60019 | -3.97081 | H                        | 6.46365  | 1.95439  | -4.71327 | C | -5.63258 | -2.94785 | -0.26139 |
| C | 0.56872  | -3.67059 | -3.02845 | H                        | 6.50144  | 3.67358  | -3.51689 | C | -4.94643 | -4.19756 | -0.23198 |
| C | -0.64844 | -4.06705 | -2.44242 | H                        | 6.54029  | 4.86135  | -1.41901 | C | -1.34312 | 4.42561  | -0.26555 |
| C | -0.64454 | -4.59345 | -1.11677 | H                        | 6.56435  | 4.98026  | 0.67304  | C | -0.61091 | 5.61463  | -0.21532 |
| C | -1.87407 | -4.67213 | -0.39667 | H                        | 6.57264  | 4.05503  | 2.89797  | C | 0.76853  | 5.61592  | -0.18646 |
| C | -3.12296 | -4.57446 | -1.09456 | C                        | -2.54226 | -0.74952 | -0.72906 | C | -2.79952 | 4.42543  | -0.30857 |
| C | -4.33514 | -4.72483 | -0.39305 | C                        | -1.60003 | -0.87197 | 0.46048  | C | -3.48890 | 3.18736  | -0.31905 |
| C | -5.53956 | -4.64988 | -1.14856 | H                        | -3.51837 | -0.37816 | -0.41098 | C | -4.91290 | 3.17753  | -0.33965 |
| C | -5.54421 | -4.12981 | -2.41404 | H                        | -2.13352 | -0.06844 | -1.48142 | C | -5.61630 | 1.94589  | -0.33579 |
| C | 0.57741  | -4.71244 | -0.42557 | H                        | -2.68134 | -1.72268 | -1.20687 | C | -7.05594 | 1.94357  | -0.35300 |
| C | 3.05494  | -4.74658 | -0.44540 | H                        | -1.49614 | 0.07353  | 1.00655  | C | -7.73450 | 0.74809  | -0.34407 |
| C | 1.80839  | -4.59448 | -1.13669 | H                        | -1.96407 | -1.60128 | 1.19587  | C | -7.04981 | -0.49347 | -0.31694 |
| C | 1.80356  | -4.06977 | -2.43757 | C                        | -0.21696 | -1.30122 | 0.03944  | C | -7.73889 | -1.70188 | -0.30544 |
| C | 3.04693  | -3.68914 | -3.04016 | O                        | 0.62008  | -1.41068 | 1.08908  | C | -7.06397 | -2.92885 | -0.27786 |
| C | 3.05044  | -2.62525 | -3.99595 | O                        | 0.13600  | -1.51825 | -1.09485 | C | -7.77591 | -4.15585 | -0.26653 |
| C | 1.81082  | -1.97673 | -4.30677 | H                        | 1.47302  | -1.71748 | 0.74106  | C | -7.09863 | -5.34710 | -0.24126 |
| C | 1.82448  | -0.62715 | -4.69176 |                          |          |          |          | C | -5.69280 | -5.36837 | -0.22458 |
| C | 3.07518  | 0.06818  | -4.77448 |                          |          |          |          | C | -5.63539 | 4.40055  | -0.36142 |
| C | 3.09690  | 1.48108  | -4.54771 | Propanoic acid-graphene, |          |          |          | C | -7.07546 | 4.37467  | -0.38276 |
| C | 1.86648  | 2.15183  | -4.24754 | gas                      |          |          |          | C | -7.75276 | 3.20676  | -0.37850 |
| C | 1.89084  | 3.31045  | -3.45479 | C                        | 3.70373  | 5.62358  | -0.16971 | C | -4.92722 | 5.60228  | -0.36283 |
| C | 3.14603  | 3.79243  | -2.95863 | C                        | 2.96202  | 4.43399  | -0.18312 | C | -3.54429 | 5.61298  | -0.33606 |
| C | 3.16911  | 4.49792  | -1.71377 | C                        | 3.65609  | 3.19835  | -0.18321 | C | -0.44440 | -0.44861 | 3.07985  |
| C | 1.93608  | 4.69980  | -1.01115 | C                        | 5.08033  | 3.19240  | -0.16457 | C | -1.10636 | 0.87374  | 2.78745  |
| C | 1.95186  | 4.78539  | 0.39010  | C                        | 5.79912  | 4.41781  | -0.14852 | C | -1.45495 | -1.57897 | 3.20067  |
| C | 3.20029  | 4.66678  | 1.08473  | C                        | 5.08695  | 5.61698  | -0.15228 | H | -7.60336 | 5.32394  | -0.40136 |
| C | 3.20506  | 4.11523  | 2.40474  | C                        | 5.78788  | 1.96274  | -0.16358 | H | 7.76454  | 5.34676  | -0.11797 |
| C | 1.96094  | 3.70281  | 2.98470  | C                        | 7.22763  | 1.96431  | -0.14602 | H | -8.82592 | -1.69548 | -0.31729 |
| C | 1.95341  | 2.65512  | 3.91861  | C                        | 7.92027  | 3.23008  | -0.12951 | H | -8.82162 | 0.74461  | -0.35594 |
| C | 3.18960  | 2.02313  | 4.27414  | C                        | 7.23930  | 4.39589  | -0.13062 | H | -8.83866 | 3.19058  | -0.39291 |
| C | 5.47905  | -4.82771 | 0.94212  | C                        | 2.94146  | 1.96101  | -0.20198 | H | -8.86146 | -4.12969 | -0.27904 |
| C | 5.46701  | -4.90805 | -0.42434 | C                        | 3.64869  | 0.74282  | -0.19968 | H | -7.64298 | -6.28571 | -0.23410 |
| C | 4.26725  | -4.70310 | -1.16210 | C                        | 5.08072  | 0.74340  | -0.17867 | H | -5.20116 | -6.33316 | -0.20664 |
| C | 4.26331  | -4.15462 | -2.50266 | C                        | 5.79202  | -0.48547 | -0.17621 | H | -3.25630 | -6.33520 | -0.14183 |
| C | 5.45979  | -3.77701 | -3.17459 | C                        | 7.22898  | -0.47349 | -0.16036 | H | -0.86204 | -6.33491 | -0.12676 |
|   |          |          |          | C                        | 7.90956  | 0.77068  | -0.14556 |   |          |          |          |

|   |          |          |          |
|---|----------|----------|----------|
| H | 1.05531  | -6.33397 | -0.19816 |
| H | 3.44982  | -6.32759 | -0.19165 |
| H | 5.39552  | -6.31985 | -0.20465 |
| H | 7.83723  | -6.26483 | -0.18712 |
| H | 9.04996  | -4.10561 | -0.16495 |
| H | 9.00812  | -1.67082 | -0.14999 |
| H | 8.99664  | 0.77062  | -0.13322 |
| H | 9.00622  | 3.21748  | -0.11615 |
| H | -5.47541 | 6.53985  | -0.38443 |
| H | -3.04243 | 6.57228  | -0.34082 |
| H | -1.11930 | 6.57011  | -0.19536 |
| H | 1.27293  | 6.57290  | -0.14635 |
| H | 3.19959  | 6.58159  | -0.17655 |
| H | 5.63237  | 6.55639  | -0.14234 |
| H | -2.10601 | -1.42689 | 4.06450  |
| H | -2.09441 | -1.61758 | 2.31551  |
| H | -0.94776 | -2.54051 | 3.30723  |
| H | 0.15049  | -0.32761 | 3.99196  |
| H | 0.27910  | -0.63014 | 2.27608  |
| O | -0.20492 | 1.87089  | 2.68376  |
| O | -2.29157 | 1.05208  | 2.64769  |
| H | -0.69739 | 2.67020  | 2.43780  |

Propanoicacid-convex  
surface of SWCNT, gas

|   |          |          |          |
|---|----------|----------|----------|
| C | 0.96150  | -4.33370 | 4.67028  |
| C | -0.20030 | -4.92872 | 4.04139  |
| C | -1.20742 | -4.08185 | 3.53861  |
| C | -1.25784 | -2.70895 | 3.94805  |
| C | -0.13220 | -2.13224 | 4.55750  |
| C | 1.04210  | -2.92984 | 4.75630  |
| C | -0.22979 | -6.29091 | 3.62906  |
| C | -0.98505 | -6.68829 | 2.55902  |
| C | -1.76403 | -5.75209 | 1.82230  |
| C | -1.99716 | -4.49703 | 2.41927  |
| C | -2.80793 | -3.52464 | 1.74717  |
| C | -3.07067 | -3.68118 | 0.37639  |
| C | -2.52343 | -4.80978 | -0.31823 |
| C | -2.03578 | -5.91363 | 0.40843  |
| C | -3.10481 | -2.28041 | 2.38078  |
| C | -2.31845 | -1.86726 | 3.49836  |
| C | -3.62690 | -2.59159 | -0.35815 |
| C | -4.18031 | -1.49196 | 0.32919  |
| C | -3.91626 | -1.33503 | 1.72342  |
| C | -4.18274 | -0.07749 | 2.34073  |
| C | -3.41376 | 0.32775  | 3.44221  |
| C | -2.37555 | -0.52459 | 3.92215  |
| C | -1.23163 | 0.06184  | 4.54249  |
| C | -0.06978 | -0.71553 | 4.71750  |
| C | -4.70752 | -0.38934 | -0.40507 |
| C | -5.28706 | 0.72311  | 0.28795  |
| C | -5.02167 | 0.88071  | 1.68367  |
| C | -5.35534 | 2.08643  | 2.33185  |
| C | -4.55988 | 2.50596  | 3.46848  |
| C | -3.49085 | 1.68892  | 3.88616  |
| C | -2.34517 | 2.27621  | 4.50988  |
| C | -1.16200 | 1.48177  | 4.66696  |
| C | -5.89135 | 1.76624  | -0.43880 |
| C | -6.50380 | 2.80838  | 0.31204  |
| C | -6.24371 | 2.96442  | 1.64869  |
| C | -2.28826 | 3.67035  | 4.70525  |
| C | -3.50505 | 4.39652  | 4.57314  |
| C | -4.60151 | 3.83456  | 3.97596  |
| C | 0.09200  | 2.11232  | 4.66914  |
| C | 0.16039  | 3.53592  | 4.51555  |
| C | -0.99329 | 4.32086  | 4.70882  |
| C | 1.20529  | -0.07446 | 4.71999  |
| C | 1.27408  | 1.32215  | 4.54710  |
| C | 2.42861  | 1.89347  | 3.93255  |
| C | 2.36726  | 3.23760  | 3.45759  |
| C | 1.31793  | 4.10831  | 3.89918  |
| C | 1.30116  | 5.45511  | 3.48599  |
| C | 0.25707  | 6.27863  | 3.99276  |
| C | -0.85003 | 5.73132  | 4.58321  |
| C | 3.16114  | 3.61926  | 2.36413  |

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.90334  | 4.87049  | 1.71417  |
| C | 2.11967  | 5.84853  | 2.35724  |
| C | 3.47449  | 1.04815  | 3.51217  |
| C | 4.28163  | 1.43622  | 2.40077  |
| C | 4.01458  | 2.65588  | 1.74805  |
| C | 4.31330  | 2.78324  | 0.35814  |
| C | 3.74906  | 3.86983  | -0.37455 |
| C | 3.20191  | 4.99781  | 0.32056  |
| C | 2.71181  | 6.10126  | -0.40501 |
| C | 2.22023  | 7.20711  | 0.34443  |
| C | 1.93429  | 7.08504  | 1.67751  |
| C | 3.48344  | 3.71328  | -1.74408 |
| C | 2.67080  | 4.68482  | -2.41530 |
| C | 2.43756  | 5.93962  | -1.81846 |
| C | 4.86879  | 1.68656  | -0.33034 |
| C | 4.59919  | 1.52776  | -1.72283 |
| C | 3.78238  | 2.47043  | -2.37806 |
| C | 2.99574  | 2.05647  | -3.49497 |
| C | 1.93428  | 2.89696  | -3.94478 |
| C | 1.88200  | 4.26962  | -3.53489 |
| C | 0.87478  | 5.11599  | -4.03828 |
| C | 0.90250  | 6.47774  | -3.62481 |
| C | 1.65731  | 6.87518  | -2.55439 |
| C | 0.81002  | 2.31957  | -4.55618 |
| C | -0.36472 | 3.11635  | -4.75682 |
| C | -0.28545 | 4.52027  | -4.66984 |
| C | 3.05488  | 0.71382  | -3.91824 |
| C | 1.91189  | 0.12670  | -4.53941 |
| C | 0.74948  | 0.90298  | -4.71652 |
| C | -0.52513 | 0.26076  | -4.72200 |
| C | -1.70159 | 1.05363  | -4.56793 |
| C | -1.64257 | 2.47259  | -4.76278 |
| C | -2.81923 | 3.24355  | -4.68121 |
| C | -2.70008 | 4.64024  | -4.92642 |
| C | -1.47743 | 5.25623  | -4.92114 |
| C | -2.83787 | 0.49079  | -3.96569 |
| C | -3.91337 | 1.34748  | -3.56009 |
| C | -3.99280 | 2.66195  | -4.06079 |
| C | -0.59245 | -1.13599 | -4.54869 |
| C | -1.74679 | -1.70791 | -3.93506 |
| C | -2.79449 | -0.86334 | -3.51804 |
| C | -3.59957 | -1.24960 | -2.40463 |
| C | -4.42491 | -0.27144 | -1.77464 |
| C | -4.72172 | 0.95944  | -2.44555 |
| C | -5.59676 | 1.89024  | -1.85211 |
| C | -5.88287 | 3.07383  | -2.58792 |
| C | -5.10815 | 3.44668  | -3.65376 |
| C | -3.32876 | -2.46682 | -1.74801 |
| C | -2.22067 | -4.68233 | -1.71135 |
| C | -2.47680 | -3.43183 | -2.36300 |
| C | -1.68369 | -3.05129 | -3.45716 |
| C | -0.63318 | -3.92148 | -3.89614 |
| C | 0.52389  | -3.34845 | -4.51291 |
| C | 0.59063  | -1.92507 | -4.66820 |
| C | 1.84393  | -1.29320 | -4.66450 |
| C | 3.02802  | -2.08574 | -4.50776 |
| C | 4.17400  | -1.49666 | -3.88543 |
| C | 4.09638  | -0.13632 | -3.44057 |
| C | 4.86984  | 0.27075  | -2.34167 |
| C | 5.71753  | -0.68344 | -1.68926 |
| C | 5.98739  | -0.52453 | -0.29288 |
| C | 5.40074  | 0.58364  | 0.40210  |
| C | 5.10682  | 0.45833  | 1.76909  |
| C | 5.39950  | -0.77476 | 2.43822  |
| C | 4.59020  | -1.16394 | 3.55222  |
| C | 3.51618  | -0.30647 | 3.95891  |
| C | 2.38060  | -0.86844 | 4.56319  |
| C | 2.32055  | -2.28705 | 4.75887  |
| C | -1.54235 | -7.01954 | -0.34010 |
| C | -1.25224 | -6.89715 | -1.67215 |
| C | -1.43524 | -5.66040 | -2.35242 |
| C | -0.61500 | -5.26745 | -3.47998 |
| C | 0.43132  | -6.09039 | -3.98348 |
| C | 1.53778  | -5.54260 | -4.57440 |
| C | 1.67883  | -4.13205 | -4.70396 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 2.97263  | -3.47987 | -4.70297 |
| C | 4.19137  | -4.20400 | -4.57513 |
| C | 5.28777  | -3.64046 | -3.98016 |
| C | 5.24445  | -2.31246 | -3.46966 |
| C | 6.04132  | -1.89305 | -2.33471 |
| C | 6.91927  | -2.78070 | -1.65116 |
| C | 7.17764  | -2.62876 | -0.31543 |
| C | 6.57661  | -1.57802 | 0.43370  |
| C | 6.27364  | -1.70679 | 1.84483  |
| C | 6.55816  | -2.89178 | 2.58015  |
| C | 5.78343  | -3.26436 | 3.64557  |
| C | 4.66880  | -2.47845 | 4.05283  |
| C | 3.49626  | -3.05907 | 4.67532  |
| C | 3.37658  | -4.45565 | 4.92172  |
| C | 2.15350  | -5.07059 | 4.91952  |
| H | 1.96444  | 8.13200  | -0.16030 |
| H | 1.45923  | 7.91631  | 2.18649  |
| H | 0.27917  | 7.34863  | 3.81891  |
| H | -1.66981 | 6.38497  | 4.85932  |
| H | -3.54231 | 5.44474  | 4.84768  |
| H | -5.47177 | 4.45548  | 3.79343  |
| H | -6.64405 | 3.83361  | 2.15872  |
| H | -7.10493 | 3.55667  | -0.19221 |
| H | -6.65508 | 3.75205  | -2.24238 |
| H | -5.29144 | 4.40871  | -4.11912 |
| H | -3.59092 | 5.25231  | -5.01248 |
| H | -1.43884 | 6.33664  | -5.00464 |
| H | 0.23837  | 7.19826  | -4.08913 |
| H | 1.56708  | 7.89762  | -2.20517 |
| H | 4.26704  | -5.06846 | 5.00643  |
| H | 2.11412  | -6.15084 | 5.00396  |
| H | 0.43351  | -7.01171 | 4.09397  |
| H | -0.89579 | -7.71098 | 2.21025  |
| H | -1.28850 | -7.94474 | 0.16508  |
| H | -0.77645 | -7.72873 | -2.18006 |
| H | 0.41130  | -7.16002 | -3.80665 |
| H | 2.35909  | -6.19549 | -4.84773 |
| H | 4.23063  | -5.25124 | -4.85345 |
| H | 6.16115  | -4.25869 | -3.80395 |
| H | 7.30879  | -3.65502 | -2.16055 |
| H | 7.76319  | -3.38796 | 0.19098  |
| H | 7.32977  | -3.57071 | 2.23460  |
| H | 5.96607  | -4.22644 | 4.11103  |
| H | -6.69548 | -4.42880 | -1.46392 |
| C | -6.97206 | -3.37857 | -1.34845 |
| H | -6.17063 | -2.76147 | -1.76425 |
| H | -7.87283 | -3.18043 | -1.93232 |
| C | -7.19946 | -3.03800 | 0.11703  |
| C | -7.54505 | -1.58038 | 0.29632  |
| H | -8.02712 | -3.61958 | 0.54099  |
| H | -6.32311 | -3.25904 | 0.73392  |
| O | -7.39799 | -1.18117 | 1.57515  |
| O | -7.91494 | -0.83471 | -0.57671 |
| H | -7.60687 | -0.23329 | 1.59600  |

Formic acid-concave  
surface of SWCNT, gas

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.51448 | 0.05025  | -4.83852 |
| C | -4.31490 | -0.70590 | -4.71640 |
| C | -3.10046 | 0.00787  | -4.71899 |
| C | -3.10341 | 1.42552  | -4.52292 |
| C | -4.32112 | 2.10517  | -4.32412 |
| C | -5.51745 | 1.40597  | -4.64841 |
| C | -1.85584 | -0.69819 | -4.63879 |
| C | -1.85141 | -2.03791 | -4.22094 |
| C | -3.09178 | -2.67258 | -3.88737 |
| C | -4.31007 | -2.09030 | -4.28944 |
| C | -3.08754 | -3.72986 | -2.92378 |
| C | -4.30345 | -4.18224 | -2.37459 |
| C | -5.50203 | -3.80109 | -3.04066 |
| C | -5.50511 | -2.79200 | -3.96552 |
| C | -1.84367 | -4.12042 | -2.32883 |
| C | -0.61028 | -3.72002 | -2.92318 |
| C | -0.61455 | -2.66412 | -3.88335 |
| C | 0.60231  | -2.04836 | -4.23907 |

|   |          |          |          |   |          |          |          |                           |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|---------------------------|----------|----------|----------|
| C | 0.59810  | -0.68508 | -4.66353 | C | -3.09663 | 4.72520  | 1.04382  | H                         | -6.45361 | 4.20190  | 2.91207  |
| C | -0.62304 | 0.01581  | -4.71842 | C | -3.09214 | 4.20124  | 2.37503  | H                         | -6.46092 | 5.08143  | 0.66856  |
| C | -0.62588 | 1.42988  | -4.52469 | C | -1.84671 | 3.78223  | 2.94772  | H                         | -6.46615 | 4.90979  | -1.42032 |
| C | -1.86181 | 2.08955  | -4.25554 | C | -1.84232 | 2.75211  | 3.90111  | H                         | -6.46914 | 3.67890  | -3.49338 |
| C | -1.84028 | -4.64557 | -1.02761 | C | -0.60525 | 2.14407  | 4.26955  | H                         | -1.11508 | -2.07157 | 0.46406  |
| C | -3.08263 | -4.76531 | -0.32235 | C | -0.60186 | 0.78047  | 4.69024  | Formic acid-graphene, gas |          |          |          |
| C | -4.30105 | -4.71452 | -1.02780 | C | 0.61849  | 0.07814  | 4.74036  | C                         | 7.79919  | -3.14551 | -0.22661 |
| C | 0.61138  | -4.12063 | -2.34500 | C | 1.85220  | 0.79050  | 4.66438  | C                         | 7.09804  | -1.88469 | -0.20341 |
| C | 0.61574  | -4.65870 | -1.02274 | C | 3.09587  | 0.08210  | 4.73851  | C                         | 5.65832  | -1.89160 | -0.20121 |
| C | -0.60333 | -4.76921 | -0.32467 | C | 4.31146  | 0.79391  | 4.73690  | C                         | 4.95911  | -3.12554 | -0.21941 |
| C | -0.60001 | -4.64150 | 1.09842  | C | 0.62028  | -1.33398 | 4.53425  | C                         | 5.68580  | -4.34617 | -0.24092 |
| C | -1.83565 | -4.39478 | 1.77154  | C | 1.85470  | -1.99438 | 4.26150  | C                         | 7.12590  | -4.31561 | -0.24477 |
| C | -3.08091 | -4.63810 | 1.10331  | C | 3.09680  | -1.33431 | 4.53479  | C                         | 4.98153  | -5.55005 | -0.25982 |
| C | -4.29539 | -4.47141 | 1.79712  | C | 4.31336  | -2.01560 | 4.33577  | C                         | 3.59843  | -5.56533 | -0.25163 |
| C | -5.49428 | -4.76667 | 1.08923  | C | 5.51063  | -1.31951 | 4.66310  | C                         | 2.84939  | -4.38033 | -0.22495 |
| C | -5.49691 | -4.88381 | -0.27442 | C | 5.50995  | 0.03573  | 4.85649  | C                         | 3.53494  | -3.14002 | -0.21585 |
| C | 1.84448  | -3.68812 | -2.91973 | C | -3.08332 | 2.14315  | 4.28059  | C                         | 2.81298  | -1.90729 | -0.20564 |
| C | 1.84005  | -2.65412 | -3.86868 | C | -3.07994 | 0.77592  | 4.70281  | C                         | 1.38043  | -1.91456 | -0.21046 |
| C | 0.61973  | -4.41957 | 1.76923  | C | -1.83565 | 0.06500  | 4.73204  | C                         | 0.67627  | -3.15700 | -0.20493 |
| C | 1.85363  | -4.62471 | 1.08411  | C | -1.83378 | -1.32434 | 4.52967  | C                         | 1.39244  | -4.38521 | -0.20252 |
| C | 1.85145  | -4.74265 | -0.31416 | C | -0.59834 | -1.99537 | 4.28653  | C                         | 3.51162  | -0.68498 | -0.18224 |
| C | 3.09265  | -4.64437 | -1.02338 | C | -0.59759 | -3.18605 | 3.49918  | C                         | 4.94311  | -0.67708 | -0.18087 |
| C | 3.08978  | -4.10947 | -2.34937 | C | 0.62052  | -3.67702 | 2.98824  | C                         | 2.80132  | 0.55226  | -0.16581 |
| C | 4.30358  | -3.74942 | -2.96645 | C | 1.85476  | -3.16618 | 3.48864  | C                         | 1.36845  | 0.54537  | -0.16603 |
| C | 4.29881  | -2.68295 | -3.94721 | C | 3.09690  | -3.67719 | 2.99093  | C                         | 0.66605  | -0.69696 | -0.19921 |
| C | 3.08042  | -2.04388 | -4.24844 | C | 4.31326  | -3.22613 | 3.54002  | C                         | -0.76560 | -0.70439 | -0.17035 |
| C | 3.07598  | -0.67869 | -4.67604 | C | 5.51083  | -4.50475 | 1.85611  | C                         | -1.46734 | -1.92857 | -0.17176 |
| C | 1.83140  | 0.03142  | -4.70969 | C | 5.51110  | -3.80222 | 3.03082  | C                         | -0.75274 | -3.16385 | -0.18452 |
| C | 1.82840  | 1.42241  | -4.51871 | C | -3.07639 | -2.00077 | 4.30036  | C                         | -1.45603 | -4.39799 | -0.17418 |
| C | 0.59241  | 2.09463  | -4.28146 | C | -3.07685 | -3.19328 | 3.50925  | C                         | -0.71599 | -5.58300 | -0.16231 |
| C | 3.09600  | -4.41622 | 1.76619  | C | -1.83423 | -3.66825 | 2.97427  | C                         | 0.66362  | -5.57711 | -0.17391 |
| C | 4.31267  | -4.68342 | 1.10932  | C | -4.29347 | -3.72674 | 3.04026  | C                         | 0.65649  | 1.76250  | -0.13830 |
| C | 4.31103  | -4.80051 | -0.33422 | C | -5.49010 | -3.24352 | 3.64062  | C                         | -0.77819 | 1.75566  | -0.12314 |
| C | 5.50738  | -4.74033 | -1.10316 | C | -5.48964 | -2.10223 | 4.39654  | C                         | -1.47885 | 0.53167  | -0.14155 |
| C | 5.50388  | -4.23329 | -2.37440 | C | -4.29319 | -1.36163 | 4.60879  | C                         | -2.91202 | 0.52567  | -0.11980 |
| C | 4.29039  | 0.02518  | -4.79582 | C | -4.29517 | 0.07235  | 4.81730  | C                         | -3.61098 | -0.71899 | -0.12871 |
| C | 5.48959  | -0.74128 | -4.79680 | C | -5.49404 | 0.83956  | 4.82262  | C                         | -2.89997 | -1.93490 | -0.14838 |
| C | 5.49355  | -2.04747 | -4.38786 | C | -5.49713 | 2.14715  | 4.41845  | C                         | -3.61082 | -3.17454 | -0.15277 |
| C | 4.28730  | 1.46068  | -4.59786 | C | -4.30174 | 2.78251  | 3.97883  | C                         | -2.91296 | -4.40787 | -0.16956 |
| C | 3.07036  | 2.10147  | -4.29391 | C | -4.30630 | 3.84563  | 2.99434  | C                         | -5.03512 | -3.17331 | -0.14086 |
| C | 0.59171  | 3.28855  | -3.49892 | C | -5.50643 | 4.32701  | 2.39945  | C                         | -5.74646 | -1.94601 | -0.11997 |
| C | 1.82714  | 3.77290  | -2.97413 | C | -5.51087 | 4.82736  | 1.12548  | C                         | -5.04311 | -0.72443 | -0.11182 |
| C | 3.06954  | 3.29749  | -3.50807 | C | -4.31529 | 4.88182  | 0.35467  | C                         | -5.75834 | 0.50196  | -0.08956 |
| C | 4.28621  | 3.82942  | -3.03747 | C | -4.31899 | 4.76363  | -1.08949 | C                         | -5.06528 | 1.73111  | -0.08070 |
| C | 5.48322  | 3.34608  | -3.63722 | C | -5.51829 | 4.58489  | -1.83474 | C                         | -3.62750 | 1.73860  | -0.09631 |
| C | 5.48363  | 2.20280  | -4.38990 | C | -5.51994 | 3.88628  | -3.01194 | C                         | -2.92903 | 2.98189  | -0.08450 |
| C | -1.86253 | 3.26379  | -3.48565 | C | -4.32219 | 3.31561  | -3.52776 | C                         | -1.50122 | 2.98844  | -0.09643 |
| C | -0.62736 | 3.77426  | -2.98521 | O | 1.15430  | -1.72162 | 0.17100  | C                         | -5.75011 | -4.40099 | -0.15063 |
| C | -0.62560 | 4.50289  | -1.75762 | C | 0.28733  | -1.46097 | -0.61895 | C                         | -5.03420 | -5.59775 | -0.17418 |
| C | 0.59490  | 4.71931  | -1.08755 | O | -1.01913 | -1.66322 | -0.41492 | C                         | -3.65090 | -5.59976 | -0.18379 |
| C | 1.82873  | 4.48850  | -1.76610 | H | 0.44901  | -1.02146 | -1.61558 | C                         | -7.18624 | -1.95238 | -0.10636 |
| C | 3.07308  | 4.72731  | -1.09613 | H | 6.44029  | 5.08516  | 0.79224  | C                         | -7.87498 | -3.22033 | -0.11666 |
| C | 4.28785  | 4.56825  | -1.79113 | H | 6.43341  | 4.89206  | -1.60950 | C                         | -7.19042 | -4.38382 | -0.13820 |
| C | 0.59862  | 4.83358  | 0.33555  | H | 6.43115  | 3.82217  | -3.41249 | C                         | -7.19525 | 0.48523  | -0.07528 |
| C | 1.83590  | 4.71193  | 1.03627  | H | 6.43170  | 1.80934  | -4.73913 | C                         | -7.87190 | -0.76111 | -0.08465 |
| C | 3.07689  | 4.84142  | 0.33060  | H | 6.43657  | -0.26294 | -5.02100 | C                         | -5.79213 | 2.94887  | -0.05805 |
| C | 4.29543  | 4.79310  | 1.03583  | H | 6.44374  | -2.56267 | -4.30245 | C                         | -7.22351 | 2.92067  | -0.04455 |
| C | 5.49032  | 4.96967  | 0.28256  | H | 6.45132  | -4.10404 | -2.88544 | C                         | -7.89131 | 1.68951  | -0.05334 |
| C | 5.48667  | 4.86069  | -1.08180 | H | 6.45731  | -4.99422 | -0.64587 | C                         | -3.64823 | 4.20772  | -0.06122 |
| C | -3.10538 | 3.76919  | -2.98144 | H | 6.45884  | -4.83331 | 1.44487  | C                         | -5.11301 | 4.20290  | -0.04874 |
| C | -3.10371 | 4.49976  | -1.75085 | H | 6.45931  | -3.59617 | 3.51476  | C                         | -5.86617 | 5.36926  | -0.02761 |
| C | -1.85928 | 4.69898  | -1.06805 | H | 6.45953  | -1.84417 | 4.65675  | C                         | -7.27181 | 5.33885  | -0.01473 |
| C | -1.85566 | 4.81171  | 0.33142  | H | 6.45875  | 0.54096  | 4.99827  | C                         | -7.94239 | 4.14357  | -0.02260 |
| C | -0.61846 | 4.72631  | 1.03761  | H | 6.45381  | 2.54179  | 4.37906  | C                         | 1.36776  | 3.00184  | -0.11166 |
| C | -0.61387 | 4.20277  | 2.36503  | H | 6.44726  | 4.31157  | 2.74335  | C                         | 0.65628  | 4.22824  | -0.08474 |
| C | 0.60753  | 3.80539  | 2.94418  | H | -6.46719 | 1.92917  | -4.64321 | C                         | -0.80099 | 4.22162  | -0.08000 |
| C | 1.84040  | 4.19635  | 2.34155  | H | -6.46248 | -0.45670 | -4.97932 | C                         | -1.54043 | 5.40538  | -0.05927 |
| C | 3.08566  | 3.81284  | 2.93894  | H | -6.45432 | -2.45984 | -4.37099 | C                         | -2.92222 | 5.39747  | -0.05048 |
| C | 4.30017  | 4.26143  | 2.38346  | H | -6.44912 | -4.23654 | -2.74187 | C                         | 2.79536  | 3.00845  | -0.11650 |
| C | 0.61195  | 2.75766  | 3.91317  | H | -6.44682 | -4.99866 | -0.78437 | C                         | 3.50307  | 4.24088  | -0.09303 |
| C | 1.84886  | 2.13149  | 4.25047  | H | -6.44137 | -4.79265 | 1.61651  | C                         | 2.76640  | 5.42388  | -0.06482 |
| C | 3.08994  | 2.76237  | 3.91026  | H | -6.43824 | -3.71889 | 3.41544  | C                         | 1.38462  | 5.41869  | -0.06064 |
| C | 4.30830  | 2.17820  | 4.30911  | H | -6.43759 | -1.70959 | 4.74707  | C                         | 3.50504  | 1.77153  | -0.13976 |
| C | 5.50369  | 2.87553  | 3.97701  | H | -6.44122 | 0.36105  | 5.04572  | C                         | 5.64695  | 0.55544  | -0.16034 |
| C | 5.49990  | 3.88066  | 3.04771  | H | -6.44687 | 2.66359  | 4.33512  |                           |          |          |          |

|                            |          |          |          |   |          |          |          |            |          |          |          |
|----------------------------|----------|----------|----------|---|----------|----------|----------|------------|----------|----------|----------|
| C                          | 4.94273  | 1.77770  | -0.13968 | C | 5.07654  | 5.13401  | -0.27205 | C          | -5.48964 | -0.64680 | 4.86818  |
| C                          | 5.65828  | 3.00190  | -0.11957 | C | -2.12644 | 3.32726  | -2.95536 | C          | 3.25590  | -2.00681 | 4.30863  |
| C                          | 4.96783  | 4.24935  | -0.09750 | C | -2.03287 | 2.30739  | -3.91619 | C          | 3.13462  | -0.64757 | 4.73933  |
| C                          | 7.77258  | -0.68706 | -0.18415 | C | -0.98124 | 4.15791  | 1.76096  | C          | 1.83404  | -0.04575 | 4.77015  |
| C                          | 7.08379  | 0.55231  | -0.16183 | C | -2.22326 | 4.24597  | 1.06728  | C          | 1.71413  | 1.33877  | 4.57058  |
| C                          | 7.76902  | 1.76276  | -0.14273 | C | -2.22576 | 4.34712  | -0.33344 | C          | 0.42622  | 1.90182  | 4.32412  |
| C                          | 7.08985  | 2.98750  | -0.12163 | C | -3.45328 | 4.15791  | -1.04853 | C          | 0.32782  | 3.07947  | 3.52395  |
| C                          | 7.79775  | 4.21672  | -0.10285 | C | -3.40280 | 3.63564  | -2.38013 | C          | -0.92592 | 3.45238  | 2.99960  |
| C                          | 7.11636  | 5.40573  | -0.08355 | C | -4.58243 | 3.18018  | -3.00189 | C          | -2.11571 | 2.84869  | 3.50487  |
| C                          | 5.71040  | 5.42249  | -0.08109 | C | -4.48597 | 2.12532  | -3.99082 | C          | -3.39399 | 3.24174  | 2.98951  |
| C                          | 0.98874  | -0.84248 | 2.81626  | C | -3.21691 | 1.59531  | -4.29754 | C          | -4.57116 | 2.69605  | 3.53848  |
| O                          | 0.19015  | -1.91347 | 2.73241  | C | -3.09508 | 0.23575  | -4.72699 | C          | -5.86172 | 3.84429  | 1.82828  |
| O                          | 2.18830  | -0.87624 | 2.77756  | C | -1.79401 | -0.36529 | -4.75786 | C          | -5.80990 | 3.16094  | 3.01352  |
| H                          | 0.38337  | 0.06950  | 2.92065  | C | -1.67310 | -1.74932 | -4.55510 | C          | 2.89519  | 2.11774  | 4.33961  |
| H                          | 7.65707  | -5.26306 | -0.26253 | C | -0.38506 | -2.31135 | -4.30747 | C          | 2.79658  | 3.29835  | 3.53681  |
| H                          | -7.71276 | -5.33633 | -0.14658 | C | -3.44814 | 3.95426  | 1.74973  | C          | 1.51993  | 3.65781  | 2.99422  |
| H                          | 8.85612  | 1.75976  | -0.14386 | C | -4.67921 | 4.11175  | 1.08325  | C          | 3.96532  | 3.92401  | 3.05962  |
| H                          | 8.85974  | -0.68017 | -0.18514 | C | -4.68208 | 4.21696  | -0.36191 | C          | 5.19701  | 3.55250  | 3.66822  |
| H                          | 8.88512  | -3.12577 | -0.22871 | C | -5.86685 | 4.05967  | -1.13422 | C          | 5.29169  | 2.42372  | 4.43634  |
| H                          | 8.88345  | 4.19402  | -0.10427 | C | -5.81893 | 3.55824  | -2.40738 | C          | 4.16155  | 1.58541  | 4.65137  |
| H                          | 7.65757  | 6.34609  | -0.06960 | C | -4.24502 | -0.56980 | -4.84330 | C          | 4.28510  | 0.15695  | 4.85791  |
| H                          | 5.21558  | 6.38567  | -0.06549 | C | -5.50557 | 0.09024  | -4.84372 | C          | 5.54506  | -0.50422 | 4.86131  |
| H                          | 3.27037  | 6.38212  | -0.04366 | C | -5.62210 | 1.39058  | -4.43189 | C          | 5.66113  | -1.80453 | 4.44956  |
| H                          | 0.87618  | 6.37385  | -0.03579 | C | -4.12001 | -1.99829 | -4.63746 | C          | 4.52519  | -2.53761 | 4.00495  |
| H                          | -1.04089 | 6.36550  | -0.05005 | C | -2.85338 | -2.52923 | -4.32430 | C          | 4.62243  | -3.59167 | 3.01563  |
| H                          | -3.43502 | 6.35108  | -0.03334 | C | -0.28590 | -3.48953 | -3.50761 | C          | 5.86010  | -3.96737 | 2.42202  |
| H                          | -5.38039 | 6.33713  | -0.02052 | C | -1.47738 | -4.07001 | -2.97898 | C          | 5.90982  | -4.46642 | 1.14830  |
| H                          | -7.82177 | 6.27411  | 0.00181  | C | -2.75382 | -3.71046 | -3.52265 | C          | 4.72529  | -4.62470 | 0.37576  |
| H                          | -9.02777 | 4.11099  | -0.01250 | C | -3.92230 | -4.33838 | -3.04848 | C          | 4.72304  | -4.51764 | -1.06919 |
| H                          | -8.97825 | 1.67647  | -0.04301 | C | -5.15356 | -3.96834 | -3.65887 | C          | 5.90544  | -4.24658 | -1.81356 |
| H                          | -8.95901 | -0.76467 | -0.07444 | C | -5.24911 | -2.83859 | -4.42543 | C          | 5.85250  | -3.56409 | -2.99904 |
| H                          | -8.96101 | -3.21127 | -0.10697 | C | 2.15710  | -3.25659 | -3.48865 | C          | 4.61286  | -3.10203 | -3.52451 |
| H                          | 5.53297  | -6.48571 | -0.28138 | C | 0.96787  | -3.86267 | -2.98409 | O          | -0.35167 | 7.54669  | -1.24676 |
| H                          | 3.09985  | -6.52617 | -0.27118 | C | 1.02320  | -4.57433 | -1.74805 | C          | -0.44347 | 7.48378  | 0.08735  |
| H                          | 1.17489  | -6.53112 | -0.15776 | C | -0.17651 | -4.88752 | -1.07869 | O          | -1.46135 | 7.29434  | 0.69503  |
| H                          | -1.21793 | -6.54179 | -0.13749 | C | -1.42301 | -4.76940 | -1.76282 | H          | 0.54739  | 7.62921  | 0.54140  |
| H                          | -3.14369 | -6.55589 | -0.20740 | C | -2.64445 | -5.10741 | -1.09348 | H          | -5.97431 | -5.73760 | 0.78968  |
| H                          | -5.57674 | -6.53880 | -0.18585 | C | -3.86624 | -5.05942 | -1.79340 | H          | -5.97784 | -5.56189 | -1.61251 |
| H                          | 0.76016  | -2.68604 | 2.58226  | C | -0.17445 | -4.99256 | 0.34496  | H          | -6.05802 | -4.52150 | -3.43150 |
| Formic acid-convex surface |          |          |          | C | -1.41903 | -4.97569 | 1.04235  | H          | -6.22619 | -2.53223 | -4.78198 |
| of SWCNT, gas              |          |          |          | C | -2.64236 | -5.21226 | 0.33397  | H          | -6.40808 | -0.46674 | -5.06881 |
| C                          | 5.52920  | 0.23833  | -4.86254 | C | -3.86246 | -5.26705 | 1.03594  | H          | -6.61290 | 1.82179  | -4.34172 |
| C                          | 4.26928  | 0.89040  | -4.74839 | C | -5.03612 | -5.54651 | 0.28088  | H          | -6.75160 | 3.35202  | -2.92050 |
| C                          | 3.11915  | 0.07609  | -4.75504 | C | -5.03806 | -5.44633 | -1.08421 | H          | -6.83569 | 4.23349  | -0.67917 |
| C                          | 3.24191  | -1.33435 | -4.54743 | C | 3.43641  | -3.64896 | -2.97497 | H          | -6.83187 | 4.08634  | 1.40864  |
| C                          | 4.51254  | -1.90621 | -4.33638 | C | 3.49176  | -4.36284 | -1.73591 | H          | -6.74037 | 2.88248  | 3.49566  |
| C                          | 5.64662  | -1.11099 | -4.66408 | C | 2.26671  | -4.65949 | -1.05363 | H          | -6.59752 | 1.14294  | 4.65934  |
| C                          | 1.81851  | 0.67460  | -4.68432 | C | 2.26878  | -4.76282 | 0.34676  | H          | -6.39218 | -1.23203 | 5.00477  |
| C                          | 1.69924  | 2.00955  | -4.26561 | C | 1.02729  | -4.78050 | 1.04955  | H          | -6.21327 | -3.22304 | 4.38316  |
| C                          | 2.88100  | 2.74317  | -3.91852 | C | 0.97501  | -4.26079 | 2.37778  | H          | -6.05098 | -4.97670 | 2.73868  |
| C                          | 4.14607  | 2.26778  | -4.31655 | C | -0.27690 | -3.97156 | 2.95607  | H          | 6.63773  | -1.55073 | -4.65263 |
| C                          | 2.78528  | 3.78295  | -2.93957 | C | -1.47043 | -4.46459 | 2.34904  | H          | 6.43127  | 0.82354  | -5.00242 |
| C                          | 3.95588  | 4.32977  | -2.37696 | C | -2.74503 | -4.19214 | 2.94541  | H          | 6.25299  | 2.81575  | -4.37877 |
| C                          | 5.18513  | 4.05754  | -3.04067 | C | -3.91566 | -4.74031 | 2.38450  | H          | 6.09117  | 4.56698  | -2.73189 |
| C                          | 5.27688  | 3.06274  | -3.97631 | C | -0.37290 | -2.93363 | 3.93136  | H          | 6.01420  | 5.32741  | -0.78104 |
| C                          | 1.51120  | 4.05184  | -2.34154 | C | -1.65953 | -2.41787 | 4.27022  | H          | 6.01957  | 5.14868  | 1.62067  |
| C                          | 0.31731  | 3.56060  | -2.94939 | C | -2.84124 | -3.15105 | 3.92267  | H          | 6.10225  | 4.10322  | 3.43800  |
| C                          | 0.41238  | 2.52489  | -3.92668 | C | -4.10636 | -2.67580 | 4.32103  | H          | 6.26896  | 2.11595  | 4.79113  |
| C                          | -0.74775 | 1.81032  | -4.28754 | C | -5.23709 | -3.47074 | 3.98132  | H          | 6.44739  | 0.05169  | 5.08982  |
| C                          | -0.62619 | 0.45357  | -4.71415 | C | -5.14505 | -4.46689 | 3.04714  | H          | 6.65157  | -2.23729 | 4.36300  |
| C                          | 0.65036  | -0.14140 | -4.76319 | C | 3.49599  | -4.56946 | 1.06161  | H          | 6.79190  | -3.76049 | 2.93642  |
| C                          | 0.77304  | -1.54823 | -4.55636 | C | 3.44377  | -4.04806 | 2.39302  | H          | 6.87913  | -4.63757 | 0.69329  |
| C                          | 2.05968  | -2.09782 | -4.27549 | C | 2.16628  | -3.73915 | 2.96501  | H          | 6.87596  | -4.48482 | -1.39263 |
| C                          | 1.46100  | 4.55415  | -1.03175 | C | 2.07210  | -2.71781 | 3.92408  | H          | 6.78250  | -3.28312 | -3.48066 |
| C                          | 2.68355  | 4.79472  | -0.32399 | C | 0.78694  | -2.21978 | 4.29386  | H          | -1.23689 | 7.35621  | -1.59755 |
| C                          | 3.90310  | 4.85361  | -1.02718 | C | 0.66578  | -0.86398 | 4.72350  | SWCNT, gas |          |          |          |
| C                          | -0.93422 | 3.84625  | -2.36820 | C | -0.61048 | -0.26856 | 4.77398  | C          | 5.50035  | -4.68907 | 1.42159  |
| C                          | -0.98537 | 4.35746  | -1.03663 | C | -1.77879 | -1.08387 | 4.69210  | C          | 4.30259  | -4.79080 | 0.65914  |
| C                          | 0.21829  | 4.55965  | -0.33234 | C | -3.07939 | -0.48508 | 4.76390  | C          | 3.08613  | -4.58711 | 1.33983  |
| C                          | 0.21939  | 4.46402  | 1.09068  | C | -4.22973 | -1.29893 | 4.75454  | C          | 3.08626  | -3.98105 | 2.63610  |
| C                          | 1.46578  | 4.35153  | 1.77503  | C | -0.73255 | 1.13899  | 4.57152  | C          | 4.30277  | -3.59046 | 3.22924  |
| C                          | 2.68635  | 4.69029  | 1.10420  | C | -2.01894 | 1.68952  | 4.29113  | C          | 5.50035  | -4.11008 | 2.66196  |
| C                          | 3.90873  | 4.64377  | 1.80361  | C | -3.20167 | 0.92590  | 4.56013  | C          | 1.84304  | -4.71637 | 0.63767  |
| C                          | 5.07946  | 5.03213  | 1.09312  | C | -4.47187 | 1.49873  | 4.34847  | C          | 0.60796  | -4.58299 | 1.34000  |
|                            |          |          |          | C | -5.60652 | 0.70299  | 4.67238  |            |          |          |          |

|   |          |          |          |   |          |          |          |               |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|---------------|----------|----------|----------|
| C | 0.60813  | -3.97783 | 2.63263  | C | -0.60792 | 4.54478  | 1.46439  | H             | 6.44856  | -4.94629 | -1.11523 |
| C | 1.84333  | -3.52461 | 3.18509  | C | -0.60816 | 3.90442  | 2.73993  | H             | 6.44889  | -3.86680 | -3.27016 |
| C | -0.61118 | -4.73210 | 0.64938  | C | 0.61084  | 3.45432  | 3.28480  | H             | 6.44865  | -2.21057 | -4.55058 |
| C | -1.84626 | -4.56341 | 1.34407  | C | 0.61041  | 2.32513  | 4.15765  | H             | 6.45025  | 0.14775  | -5.05182 |
| C | -1.84602 | -3.96837 | 2.61533  | C | -0.60891 | 1.68431  | 4.45467  | H             | 6.45061  | 2.18318  | -4.56201 |
| C | -0.61085 | -3.54305 | 3.18958  | C | -0.60947 | 0.28828  | 4.75206  | H             | 6.45165  | 4.04997  | -3.03662 |
| C | -3.08943 | -4.73472 | 0.65122  | C | 0.60931  | -0.41819 | 4.74270  | H             | 6.45217  | 4.94068  | -1.13682 |
| C | -4.30600 | -4.63884 | 1.35521  | C | 0.60878  | -1.80592 | 4.40765  | H             | 6.45193  | 4.90659  | 1.27205  |
| C | -4.30577 | -4.02470 | 2.66745  | C | -0.61044 | -2.43818 | 4.09304  | H             | 6.45171  | 3.96424  | 3.14484  |
| C | -3.08878 | -3.54615 | 3.19143  | C | 1.84302  | -4.69708 | -0.76607 | H             | 6.45037  | 2.05748  | 4.61926  |
| C | -3.08835 | -2.43838 | 4.09725  | C | 3.08605  | -4.54911 | -1.46452 | graphene, gas |          |          |          |
| C | -4.30456 | -1.82858 | 4.46287  | C | 3.08617  | -3.90760 | -2.74366 | C             | 8.87129  | -4.11941 | 0.00000  |
| C | -5.50245 | -2.54226 | 4.17714  | C | 1.84335  | -3.43609 | -3.27976 | C             | 7.15755  | -2.89344 | 0.00000  |
| C | -5.50304 | -3.60164 | 3.31041  | C | 1.84363  | -2.32578 | -4.13865 | C             | 5.72597  | -2.91500 | 0.00000  |
| C | -1.84518 | -1.78991 | 4.39484  | C | 3.08668  | -1.68808 | -4.45853 | C             | 5.04123  | -4.16602 | 0.00000  |
| C | -1.84469 | -0.42533 | 4.72449  | C | 3.08728  | -0.28825 | -4.75651 | C             | 5.78959  | -5.33572 | 0.00000  |
| C | -3.08728 | 0.28810  | 4.75666  | C | 1.84467  | 0.42522  | -4.72437 | C             | 7.19556  | -5.31177 | 0.00000  |
| C | -4.30412 | -0.42000 | 4.80297  | C | 1.84514  | 1.78981  | -4.39486 | C             | 7.83101  | -1.66537 | 0.00000  |
| C | -3.08665 | 1.68795  | 4.45864  | C | 3.08830  | 2.43823  | -4.09747 | C             | 7.14044  | -0.45806 | 0.00000  |
| C | -4.30292 | 2.35460  | 4.21184  | C | 3.08874  | 3.54591  | -3.19179 | C             | 5.70340  | -0.46799 | 0.00000  |
| C | -5.50074 | 1.68520  | 4.59021  | C | 1.84599  | 3.96815  | -2.61564 | C             | 5.00468  | -1.69387 | 0.00000  |
| C | -5.50150 | 0.34625  | 4.87502  | C | 1.84626  | 4.56342  | -1.34412 | C             | 3.57607  | -4.16416 | 0.00000  |
| C | -1.84359 | 2.32575  | 4.13869  | C | 3.08943  | 4.73480  | -0.65123 | C             | 2.86249  | -2.93491 | 0.00000  |
| C | -1.84332 | 3.43617  | 3.27974  | C | 3.08935  | 4.71503  | 0.77993  | C             | 3.56664  | -1.69473 | 0.00000  |
| C | -3.08613 | 3.90768  | 2.74364  | C | 1.84624  | 4.52505  | 1.46782  | C             | 1.43451  | -2.93451 | 0.00000  |
| C | -4.30268 | 3.50095  | 3.32582  | C | 1.84602  | 3.89536  | 2.72250  | C             | 0.72873  | -4.16454 | 0.00000  |
| C | -3.08602 | 4.54915  | 1.46452  | C | 3.08869  | 3.45735  | 3.28692  | C             | 1.46264  | -5.35188 | 0.00000  |
| C | -4.30251 | 4.77103  | 0.78977  | C | 3.08828  | 2.32531  | 4.16220  | C             | 2.84456  | -5.35072 | 0.00000  |
| C | -5.50013 | 4.64931  | 1.54922  | C | 1.84511  | 1.66900  | 4.44198  | C             | 2.85667  | -0.47844 | 0.00000  |
| C | -5.50018 | 4.03644  | 2.77316  | C | 1.84455  | 0.29588  | 4.73464  | C             | 1.42341  | -0.47765 | 0.00000  |
| C | -1.84300 | 4.69710  | 0.76606  | C | 3.08718  | -0.41810 | 4.74765  | C             | 0.71734  | -1.69821 | 0.00000  |
| C | -1.84304 | 4.71634  | -0.63770 | C | 3.08664  | -1.80946 | 4.41172  | C             | -0.71734 | -1.69821 | 0.00000  |
| C | -3.08615 | 4.58708  | -1.33984 | C | 1.84358  | -2.43829 | 4.07413  | C             | -1.43451 | -2.93451 | 0.00000  |
| C | -4.30260 | 4.79082  | -0.65911 | C | 4.30253  | -4.77102 | -0.78975 | C             | -0.72873 | -4.16454 | 0.00000  |
| C | -3.08629 | 3.98108  | -2.63604 | C | 5.50015  | -4.64933 | -1.54919 | C             | -2.86249 | -2.93491 | 0.00000  |
| C | -4.30280 | 3.59047  | -3.22921 | C | 5.50021  | -4.03640 | -2.77316 | C             | -3.57607 | -4.16416 | 0.00000  |
| C | -5.50036 | 4.11005  | -2.66200 | C | 4.30272  | -3.50088 | -3.32585 | C             | -2.84456 | -5.35072 | 0.00000  |
| C | -5.50036 | 4.68913  | -1.42154 | C | 4.30296  | -2.35469 | -4.21180 | C             | -1.46264 | -5.35188 | 0.00000  |
| C | -1.84337 | 3.52463  | -3.18502 | C | 5.50078  | -1.68543 | -4.59006 | C             | -3.56665 | -1.69473 | 0.00000  |
| C | -1.84361 | 2.43831  | -4.07403 | C | 5.50150  | -0.34652 | -4.87482 | C             | -2.85667 | -0.47844 | 0.00000  |
| C | -3.08667 | 1.80951  | -4.41157 | C | 4.30409  | 0.41985  | -4.80289 | C             | -1.42341 | -0.47765 | 0.00000  |
| C | -4.30291 | 2.46894  | -4.14650 | C | 4.30448  | 1.82845  | -4.46304 | C             | -0.71594 | 0.76208  | 0.00000  |
| C | -3.08717 | 0.41814  | -4.74753 | C | 5.50239  | 2.54214  | -4.17738 | C             | 0.71594  | 0.76208  | 0.00000  |
| C | -4.30402 | -0.28852 | -4.81304 | C | 5.50303  | 3.60156  | -3.31051 | C             | -5.04123 | -4.16602 | 0.00000  |
| C | -5.50137 | 0.47967  | -4.86440 | C | 4.30576  | 4.02458  | -2.66763 | C             | -5.72597 | -2.91500 | 0.00000  |
| C | -5.50071 | 1.80992  | -4.54285 | C | 4.30600  | 4.63889  | -1.35523 | C             | -5.00468 | -1.69387 | 0.00000  |
| C | -1.84454 | -0.29583 | -4.73455 | C | 5.50343  | 4.86053  | -0.61804 | C             | -5.70340 | -0.46799 | 0.00000  |
| C | -1.84509 | -1.66882 | -4.44205 | C | 5.50337  | 4.84147  | 0.75064  | C             | -4.99399 | 0.76191  | 0.00000  |
| C | -3.08826 | -2.32510 | -4.16228 | C | 4.30580  | 4.60016  | 1.48116  | C             | -3.56162 | 0.76317  | 0.00000  |
| C | -4.30447 | -1.70572 | -4.51104 | C | 4.30559  | 3.95016  | 2.77596  | C             | -2.85668 | 1.98256  | 0.00000  |
| C | -3.08867 | -3.45727 | -3.28693 | C | 5.50295  | 3.50937  | 3.40675  | C             | -1.42329 | 1.98331  | 0.00000  |
| C | -4.30558 | -3.95009 | -2.77596 | C | 5.50226  | 2.42691  | 4.24456  | C             | -7.15755 | -2.89344 | 0.00000  |
| C | -5.50294 | -3.50931 | -3.40673 | C | 4.30449  | 1.70587  | 4.51102  | C             | -7.87129 | -4.11941 | 0.00000  |
| C | -5.50225 | -2.42684 | -4.24452 | C | 4.30403  | 0.28861  | 4.81309  | C             | -7.19556 | -5.31177 | 0.00000  |
| C | -1.84600 | -3.89530 | -2.72251 | C | 5.50138  | -0.47959 | 4.86448  | C             | -5.78959 | -5.33572 | 0.00000  |
| C | -1.84622 | -4.52498 | -1.46784 | C | 5.50069  | -1.80984 | 4.54299  | C             | -7.83101 | -1.66537 | 0.00000  |
| C | -3.08934 | -4.71493 | -0.77994 | C | 4.30288  | -2.46888 | 4.14662  | C             | -7.14044 | -0.45806 | 0.00000  |
| C | -4.30578 | -4.60008 | -1.48117 | H | -6.44852 | 4.94616  | 1.11525  | C             | -5.70308 | 1.98015  | 0.00000  |
| C | -5.50341 | -4.86043 | 0.61805  | H | -6.44884 | 3.86683  | 3.27019  | C             | -7.14317 | 1.97949  | 0.00000  |
| C | -5.50335 | -4.84136 | -0.75064 | H | -6.44860 | 2.21026  | 4.55075  | C             | -7.82314 | 0.78510  | 0.00000  |
| C | -0.61118 | -4.71219 | -0.77805 | H | -6.45027 | -0.14813 | 5.05211  | C             | -3.57322 | 3.21902  | 0.00000  |
| C | 0.60794  | -4.54472 | -1.46440 | H | -6.45068 | -2.18328 | 4.56180  | C             | -4.99759 | 3.21103  | 0.00000  |
| C | 0.60819  | -3.90433 | -2.73996 | H | -6.45157 | -4.04985 | 3.03680  | C             | -5.71829 | 4.43537  | 0.00000  |
| C | -0.61081 | -3.45423 | -3.28482 | H | -6.45215 | -4.94058 | 1.13682  | C             | -7.15884 | 4.41150  | 0.00000  |
| C | -0.61037 | -2.32498 | -4.15772 | H | -6.45190 | -4.90645 | -1.27204 | C             | -7.83823 | 3.24432  | 0.00000  |
| C | 0.60894  | -1.68430 | -4.45464 | H | -6.45170 | -3.96420 | -3.14479 | C             | -5.00808 | 5.63551  | 0.00000  |
| C | 0.60948  | -0.28835 | -4.75192 | H | -6.45037 | -2.05748 | -4.61917 | C             | -3.62468 | 5.64405  | 0.00000  |
| C | -0.60932 | 0.41817  | -4.74255 | H | -6.45012 | -0.00943 | -5.05494 | C             | -2.88097 | 4.45569  | 0.00000  |
| C | -0.60881 | 1.80591  | -4.40754 | H | -6.44881 | 2.33345  | -4.48952 | C             | -1.42379 | 4.45299  | 0.00000  |
| C | 0.61039  | 2.43811  | -4.09309 | H | -6.44917 | 3.95416  | -3.16327 | C             | -0.71408 | 3.22232  | 0.00000  |
| C | 0.61080  | 3.54290  | -3.18980 | H | -6.44866 | 4.97402  | -0.97949 | C             | 0.71408  | 3.22232  | 0.00000  |
| C | -0.60817 | 3.97777  | -2.63271 | H | 6.45013  | 0.00952  | 5.05497  | C             | 1.42329  | 1.98331  | 0.00000  |
| C | -0.60797 | 4.58294  | -1.34006 | H | 6.44876  | -2.33332 | 4.48967  | C             | 1.42379  | 4.45299  | 0.00000  |
| C | 0.61119  | 4.73213  | -0.64941 | H | 6.44916  | -3.95425 | 3.16315  | C             | 0.68991  | 5.64130  | 0.00000  |
| C | 0.61120  | 4.71226  | 0.77803  | H | 6.44863  | -4.97387 | 0.97961  |               |          |          |          |

|   |          |          |         |
|---|----------|----------|---------|
| C | -0.68991 | 5.64130  | 0.00000 |
| C | 2.88097  | 4.45569  | 0.00000 |
| C | 3.57322  | 3.21902  | 0.00000 |
| C | 2.85668  | 1.98256  | 0.00000 |
| C | 4.99759  | 3.21103  | 0.00000 |
| C | 5.71829  | 4.43537  | 0.00000 |
| C | 5.00808  | 5.63551  | 0.00000 |
| C | 3.62468  | 5.64405  | 0.00000 |
| C | 7.15884  | 4.41150  | 0.00000 |
| C | 7.83823  | 3.24432  | 0.00000 |
| C | 7.14317  | 1.97949  | 0.00000 |
| C | 5.70308  | 1.98015  | 0.00000 |
| H | -7.68511 | 5.36191  | 0.00000 |
| H | 7.68511  | 5.36191  | 0.00000 |
| C | 7.82314  | 0.78510  | 0.00000 |
| C | 3.56162  | 0.76317  | 0.00000 |
| C | 4.99399  | 0.76191  | 0.00000 |
| H | -8.91809 | -1.65735 | 0.00000 |
| H | -8.91032 | 0.78318  | 0.00000 |
| H | -8.92426 | 3.22930  | 0.00000 |
| H | -8.95688 | -4.09120 | 0.00000 |
| H | -7.74152 | -6.24952 | 0.00000 |
| H | -5.29972 | -6.30156 | 0.00000 |
| H | -3.35305 | -6.30682 | 0.00000 |
| H | -0.95839 | -6.30961 | 0.00000 |
| H | 0.95839  | -6.30961 | 0.00000 |
| H | 3.35305  | -6.30682 | 0.00000 |
| H | 5.29972  | -6.30156 | 0.00000 |
| H | 7.74152  | -6.24952 | 0.00000 |
| H | 8.95688  | -4.09120 | 0.00000 |
| H | 8.91809  | -1.65735 | 0.00000 |
| H | 8.91032  | 0.78318  | 0.00000 |
| H | 8.92426  | 3.22930  | 0.00000 |
| H | -5.55508 | 6.57405  | 0.00000 |
| H | -3.12180 | 6.60274  | 0.00000 |
| H | -1.19635 | 6.59801  | 0.00000 |
| H | 1.19635  | 6.59801  | 0.00000 |
| H | 3.12180  | 6.60274  | 0.00000 |
| H | 5.55508  | 6.57405  | 0.00000 |

Toluene-concave surface of  
SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.47918  | 4.85023  | 1.18003  |
| C | 4.28188  | 4.52991  | 1.88144  |
| C | 3.06385  | 4.70764  | 1.19577  |
| C | 3.06237  | 4.86702  | -0.22702 |
| C | 4.28058  | 4.83240  | -0.93399 |
| C | 5.47880  | 4.99600  | -0.18141 |
| C | 1.82211  | 4.44374  | 1.86042  |
| C | 0.58560  | 4.69316  | 1.19260  |
| C | 0.58317  | 4.85858  | -0.22634 |
| C | 1.81929  | 4.75947  | -0.93458 |
| C | -0.63146 | 4.45360  | 1.86125  |
| C | -1.86844 | 4.66878  | 1.18396  |
| C | -1.87107 | 4.82533  | -0.21165 |
| C | -0.63678 | 4.77059  | -0.92797 |
| C | -3.10963 | 4.45041  | 1.86812  |
| C | -4.32922 | 4.73170  | 1.22180  |
| C | -4.33303 | 4.88197  | -0.21985 |
| C | -3.11665 | 4.74554  | -0.91744 |
| C | -3.11598 | 4.23533  | -2.25352 |
| C | -4.33171 | 3.87184  | -2.86508 |
| C | -5.53306 | 4.34403  | -2.26343 |
| C | -5.53380 | 4.83272  | -0.98428 |
| C | -1.86949 | 3.82876  | -2.83460 |
| C | -1.86468 | 2.78503  | -3.77373 |
| C | -3.10536 | 2.16978  | -4.14789 |
| C | -4.32600 | 2.80680  | -3.84811 |
| C | -3.10004 | 0.80238  | -4.56964 |
| C | -4.31547 | 0.10037  | -4.69606 |
| C | -5.51635 | 0.86483  | -4.69737 |
| C | -5.52181 | 2.17134  | -4.28715 |
| C | -1.85516 | 0.09283  | -4.59950 |
| C | -1.85281 | -1.30123 | -4.42998 |
| C | -3.09608 | -1.98568 | -4.22917 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -4.31345 | -1.33809 | -4.51884 |
| C | -3.09732 | -3.20551 | -3.48076 |
| C | -4.31582 | -3.74896 | -3.02711 |
| C | -5.51366 | -3.24752 | -3.61088 |
| C | -5.51195 | -2.08303 | -4.33203 |
| C | -1.85476 | -3.70481 | -2.96700 |
| C | -1.85638 | -4.46582 | -1.78645 |
| C | -3.10089 | -4.70658 | -1.11639 |
| C | -4.31773 | -4.52247 | -1.80132 |
| C | -3.09988 | -4.84074 | 0.30820  |
| C | -4.31577 | -4.79076 | 1.01811  |
| C | -5.51624 | -4.95250 | 0.26886  |
| C | -5.51722 | -4.82160 | -1.09433 |
| C | -1.85396 | -4.72106 | 1.00749  |
| C | -1.85172 | -4.20157 | 2.31135  |
| C | -3.09377 | -3.81835 | 2.91685  |
| C | -4.31250 | -4.26551 | 2.36886  |
| C | -3.09256 | -2.77237 | 3.89327  |
| C | -4.30962 | -2.19358 | 4.30563  |
| C | -5.50807 | -2.88838 | 3.97679  |
| C | -5.50954 | -3.88925 | 3.04164  |
| C | -1.84923 | -2.14357 | 4.23014  |
| C | -1.85019 | -0.80834 | 4.66312  |
| C | -3.09444 | -0.10230 | 4.75724  |
| C | -4.31062 | -0.81409 | 4.75097  |
| C | -3.09724 | 1.31807  | 4.57975  |
| C | -4.31617 | 2.00134  | 4.39852  |
| C | -5.51267 | 1.29969  | 4.71954  |
| C | -5.50997 | -0.05944 | 4.89041  |
| C | -1.85600 | 1.98456  | 4.31525  |
| C | -1.86013 | 3.17253  | 3.56633  |
| C | -3.10547 | 3.68994  | 3.08059  |
| C | -4.32049 | 3.22667  | 3.62393  |
| C | -5.52602 | 4.53609  | 1.96781  |
| C | -5.52186 | 3.80923  | 3.12869  |
| C | -0.62743 | 3.69218  | 3.06927  |
| C | 0.59407  | 3.19478  | 3.56555  |
| C | 0.59867  | 1.98695  | 4.32633  |
| C | -0.61889 | 1.31983  | 4.56710  |
| C | -0.61584 | -0.09674 | 4.74303  |
| C | 0.60473  | -0.79740 | 4.67126  |
| C | 0.60532  | -2.15497 | 4.23168  |
| C | -0.61416 | -2.76568 | 3.87821  |
| C | -0.61534 | -3.81090 | 2.90622  |
| C | 0.60261  | -4.21202 | 2.32202  |
| C | 0.60052  | -4.74805 | 0.99887  |
| C | -0.61997 | -4.85446 | 0.30171  |
| C | -0.62056 | -4.73222 | -1.12262 |
| C | 0.59931  | -4.50547 | -1.79365 |
| C | 0.60020  | -3.72276 | -2.98961 |
| C | -0.61818 | -3.20694 | -3.47608 |
| C | -0.61853 | -1.98009 | -4.20583 |
| C | 0.59966  | -1.30853 | -4.42451 |
| C | 0.59732  | 0.10757  | -4.59334 |
| C | -0.62291 | 0.80878  | -4.54371 |
| C | -0.62645 | 2.17618  | -4.13582 |
| C | 0.58992  | 2.80079  | -3.79566 |
| C | 0.58584  | 3.87002  | -2.84891 |
| C | -0.63533 | 4.26890  | -2.26666 |
| C | 1.82665  | 3.69308  | 3.04751  |
| C | 3.07191  | 3.20632  | 3.56476  |
| C | 3.07696  | 1.99285  | 4.32379  |
| C | 1.83596  | 1.31074  | 4.54539  |
| C | 1.83908  | -0.08286 | 4.71741  |
| C | 3.08314  | -0.79344 | 4.66738  |
| C | 3.08360  | -2.15591 | 4.22988  |
| C | 1.84005  | -2.76138 | 3.85280  |
| C | 1.83841  | -3.79149 | 2.89891  |
| C | 3.08071  | -4.21750 | 2.32526  |
| C | 3.07886  | -4.75270 | 0.99809  |
| C | 1.83558  | -4.84520 | 0.28915  |
| C | 1.83523  | -4.72413 | -1.11136 |
| C | 3.07921  | -4.49810 | -1.78884 |
| C | 3.07866  | -3.71439 | -2.98726 |
| C | 1.83473  | -3.18725 | -3.46544 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 1.83421  | -1.97902 | -4.18140 |
| C | 3.07512  | -1.30793 | -4.43157 |
| C | 3.07300  | 0.11284  | -4.60375 |
| C | 1.82976  | 0.82056  | -4.51821 |
| C | 1.82619  | 2.16704  | -4.12195 |
| C | 3.06871  | 2.80123  | -3.79467 |
| C | 3.06595  | 3.86772  | -2.84076 |
| C | 1.82070  | 4.26211  | -2.24828 |
| C | 4.28672  | 3.75192  | 3.10415  |
| C | 5.48866  | 3.25368  | 3.68311  |
| C | 5.49317  | 2.09158  | 4.40809  |
| C | 4.29645  | 1.34676  | 4.60787  |
| C | 4.29984  | -0.09216 | 4.78522  |
| C | 5.50004  | -0.85802 | 4.77002  |
| C | 5.50039  | -2.16254 | 4.35297  |
| C | 4.30056  | -2.79507 | 3.91977  |
| C | 4.29845  | -3.86217 | 2.93874  |
| C | 5.49643  | -4.35447 | 2.34662  |
| C | 5.49586  | -4.85997 | 1.07410  |
| C | 4.29665  | -4.90971 | 0.30699  |
| C | 4.29704  | -4.77229 | -1.13546 |
| C | 5.49734  | -4.56808 | -1.87411 |
| C | 5.49633  | -3.82564 | -3.02446 |
| C | 4.29567  | -3.23528 | -3.51271 |
| C | 4.29389  | -1.99449 | -4.26130 |
| C | 5.49102  | -1.29083 | -4.57425 |
| C | 5.48888  | 0.06880  | -4.74158 |
| C | 4.28965  | 0.82379  | -4.60594 |
| C | 4.28734  | 2.21059  | -4.18560 |
| C | 5.48551  | 2.90968  | -3.86459 |
| C | 5.48379  | 3.92503  | -2.94580 |
| C | 4.28281  | 4.31162  | -2.28570 |
| C | 1.45766  | 1.11854  | -0.75801 |
| C | 2.12548  | -0.09688 | -0.62784 |
| C | 1.39501  | -1.28360 | -0.62200 |
| C | 0.00878  | -1.25326 | -0.76426 |
| C | -0.67097 | -0.04237 | -0.91839 |
| C | 0.07071  | 1.14136  | -0.89799 |
| H | 3.20626  | -0.12003 | -0.52638 |
| H | 1.90816  | -2.23422 | -0.50769 |
| H | -0.56097 | -2.17966 | -0.75891 |
| C | -2.17110 | -0.01315 | -1.06919 |
| H | -0.45061 | 2.09041  | -0.99362 |
| H | -2.49414 | 0.87636  | -1.62028 |
| H | -2.53095 | -0.89939 | -1.60328 |
| H | -2.66456 | 0.00572  | -0.09096 |
| H | 2.01750  | 2.05030  | -0.75207 |
| H | -6.46263 | -3.72730 | -3.40004 |
| H | -6.45971 | -1.68113 | -4.67147 |
| H | -6.46311 | 0.38793  | -4.92415 |
| H | -6.47299 | 2.68416  | -4.20218 |
| H | -6.48244 | 4.21987  | -2.77162 |
| H | -6.48311 | 5.07663  | -0.52095 |
| H | -6.47608 | 4.87141  | 1.56773  |
| H | -6.46902 | 3.59222  | 3.60929  |
| H | -6.46229 | 1.82255  | 4.72942  |
| H | -6.45805 | -0.56579 | 5.03098  |
| H | -6.45631 | -2.55928 | 4.38630  |
| H | -6.45871 | -4.31913 | 2.74232  |
| H | -6.46523 | -5.06980 | 0.77941  |
| H | -6.46640 | -4.83861 | -1.61786 |
| H | 6.43526  | 2.57165  | -4.26309 |
| H | 6.43195  | 4.35607  | -2.64506 |
| H | 6.42694  | 5.12862  | -0.68975 |
| H | 6.42707  | 4.87369  | 1.70562  |
| H | 6.43586  | 3.73363  | 3.46492  |
| H | 6.44368  | 1.69151  | 4.74208  |
| H | 6.44957  | -0.38296 | 4.98909  |
| H | 6.45070  | -2.67500 | 4.25690  |
| H | 6.44520  | -4.23632 | 2.85741  |
| H | 6.44370  | -5.12105 | 0.61711  |
| H | 6.44627  | -4.90471 | -1.47248 |
| H | 6.44487  | -3.59967 | -3.49811 |
| H | 6.44043  | -1.81399 | -4.58659 |
| H | 6.43717  | 0.57472  | -4.88221 |

# Toluene-graphene, CPCM

C 5.13393 0.75123 -0.19645  
C 5.83626 -0.48273 -0.16182  
C 7.27297 -0.48043 -0.11337  
C 7.96408 0.75910 -0.10665  
C 7.29018 1.95759 -0.14471  
C 5.85032 1.96574 -0.18947  
C 5.13041 -1.70497 -0.17470  
C 5.84420 -2.93032 -0.13880  
C 7.27552 -2.91643 -0.08477  
C 7.95741 -1.69195 -0.07480  
C 5.15240 -4.17814 -0.15358  
C 5.89251 -5.35259 -0.10582  
C 7.29863 -5.33585 -0.05095  
C 7.98224 -4.14703 -0.04215  
C 3.69293 -1.69798 -0.22456  
C 2.98218 -2.93465 -0.24401  
C 3.68826 -4.16880 -0.21746  
C 3.70194 0.76042 -0.24132  
C 2.98979 -0.47769 -0.25372  
C 1.55488 -2.92603 -0.29707  
C 0.84336 -4.15342 -0.31618  
C 1.56990 -5.34577 -0.30728  
C 2.95200 -5.35233 -0.25903  
C 0.84456 -1.68581 -0.32981  
C 1.55715 -0.46927 -0.30702  
C -0.58878 -1.67827 -0.38997  
C -1.31136 -2.91086 -0.39543  
C -0.61416 -4.14504 -0.34849  
C 3.00436 1.98397 -0.27162  
C 1.57123 1.99233 -0.31317  
C 0.85697 0.77479 -0.32880  
C -0.57400 0.78164 -0.37319  
C -1.28758 -0.45450 -0.39413  
C -2.71961 -0.44769 -0.42169  
C -3.43559 -1.66008 -0.43103  
C -2.73865 -2.90393 -0.42517  
C -3.45869 -4.13010 -0.41597  
C -2.73635 -5.32117 -0.35047  
C -1.35383 -5.32917 -0.31614  
C -4.87372 -1.65216 -0.42198  
C -5.60199 -2.86936 -0.44065  
C -4.92346 -4.12417 -0.45700  
C -5.56674 -0.42306 -0.38927  
C -4.85013 0.80291 -0.36741  
C -3.41765 0.79659 -0.38456  
C -2.70675 2.01263 -0.35914  
C -1.27366 2.00670 -0.36289  
C -0.55857 3.24316 -0.34552  
C 0.86956 3.23649 -0.33128  
C -7.03392 -2.84055 -0.44701  
C -7.75454 -4.06327 -0.48668  
C -7.08348 -5.25877 -0.52112  
C -5.67657 -5.29023 -0.50664  
C -7.70271 -1.60932 -0.41399  
C -7.00397 -0.40567 -0.38018  
C -7.68179 0.84039 -0.33879  
C -6.99412 2.03137 -0.30871  
C -5.55362 2.02423 -0.32423  
C -4.84158 3.25193 -0.29883  
C -3.41674 3.25286 -0.31728  
C -2.71873 4.48690 -0.29909  
C -1.26116 4.47789 -0.32417  
C -5.55655 4.47953 -0.25610  
C -6.99788 4.46311 -0.23741  
C -7.68340 3.29932 -0.26304  
C -3.45612 5.67929 -0.25387  
C -4.84014 5.67715 -0.23278  
C 1.58559 4.46380 -0.31925  
C 0.85862 5.65735 -0.32070  
C -0.52195 5.66414 -0.32054  
C 3.04321 4.45818 -0.29706  
C 3.72780 3.21699 -0.26527  
C 5.15205 3.20090 -0.22665

C 5.88032 4.42157 -0.22452  
C 5.17744 5.62654 -0.26481  
C 3.79363 5.64315 -0.30009  
C 7.99311 3.21893 -0.14182  
C 7.32088 4.39009 -0.18097  
H -7.51935 5.41522 -0.20239  
H 7.85288 5.33697 -0.17956  
H -8.78943 -1.59562 -0.41392  
H -8.76863 0.84397 -0.33000  
H -8.76917 3.29004 -0.24964  
H -8.83978 -4.03023 -0.49283  
H -7.63272 -6.19355 -0.55887  
H -5.19206 -6.25824 -0.54013  
H -3.24922 -6.27411 -0.31341  
H -0.85758 -6.28889 -0.25252  
H 1.06295 -6.30122 -0.34431  
H 3.45331 -6.31206 -0.25663  
H 5.39839 -6.31619 -0.10778  
H 7.83730 -6.27686 -0.01521  
H 9.06700 -4.12539 -0.00086  
H 9.04352 -1.68998 -0.03611  
H 9.05037 0.75133 -0.07158  
H 9.07831 3.19864 -0.10812  
H -5.38116 6.61811 -0.19760  
H -2.94992 6.63590 -0.23152  
H -1.02190 6.62410 -0.31573  
H 1.36818 6.61222 -0.31267  
H 3.29836 6.60521 -0.33191  
H 5.72890 6.56207 -0.26712  
C -1.85261 -1.98427 2.81800  
C -0.50541 -1.62337 2.84364  
C -0.14292 -0.28051 2.87528  
C -1.11515 0.72594 2.88635  
C -2.46040 0.35257 2.86091  
C -2.82875 -0.99190 2.82920  
H 0.26373 -2.39068 2.81081  
H 0.90893 -0.00274 2.87407  
C -0.71355 2.17773 2.93024  
H -3.22704 1.12436 2.84717  
H -3.88048 -1.26238 2.78901  
H -1.49576 2.81715 2.51054  
H -0.53008 2.50387 3.95980  
H 0.20677 2.34547 2.36185  
H -2.13680 -3.03164 2.76971

# Toluene-convex surface of SWCNT, CPCM

C -3.66701 -5.81848 -1.82264  
C -3.33646 -4.60549 -2.49153  
C -3.70060 -3.39938 -1.86033  
C -4.06985 -3.40076 -0.47713  
C -4.07540 -4.60928 0.24760  
C -4.02484 -5.82009 -0.50071  
C -3.43779 -2.14577 -2.50466  
C -3.87206 -0.92658 -1.90148  
C -4.22807 -0.92776 -0.52013  
C -4.16293 -2.14878 0.21483  
C -3.62975 0.30194 -2.54896  
C -4.02833 1.52240 -1.92705  
C -4.37802 1.51933 -0.56855  
C -4.33862 0.29780 0.16391  
C -3.80524 2.77441 -2.58948  
C -4.26965 3.97117 -2.00801  
C -4.64563 3.96569 -0.60684  
C -4.52229 2.76683 0.12183  
C -4.27077 2.80920 1.52926  
C -4.13440 4.05081 2.18205  
C -4.58540 5.20719 1.48395  
C -4.83391 5.16525 0.13691  
C -3.88465 1.60188 2.19827  
C -3.06275 1.67854 3.33379  
C -2.62683 2.96391 3.79531  
C -3.28058 4.13092 3.35123  
C -1.36596 3.06270 4.46569  
C -0.78315 4.32768 4.68088

C -1.61952 5.46871 4.51929  
C -2.82535 5.37399 3.87625  
C -0.58672 1.87325 4.65118  
C 0.81287 1.97200 4.70114  
C 1.42943 3.25959 4.56776  
C 0.66174 4.42920 4.73503  
C 2.73725 3.34145 3.99180  
C 3.25300 4.59130 3.59546  
C 2.59310 5.75482 4.08360  
C 1.34145 5.67675 4.63384  
C 3.38331 2.13308 3.56993  
C 4.29765 2.17982 2.50549  
C 4.56297 3.43441 1.86425  
C 4.19594 4.63952 2.49557  
C 4.93527 3.43781 0.48211  
C 4.93388 4.64604 -0.24305  
C 4.87901 5.85675 0.50464  
C 4.52279 5.85347 1.82689  
C 5.03001 2.18620 -0.21060  
C 4.77534 2.14461 -1.59084  
C 4.42685 3.35526 -2.27528  
C 4.67191 4.60311 -1.66823  
C 3.58381 3.27712 -3.42931  
C 3.00213 4.44812 -3.95482  
C 3.53629 5.69468 -3.52025  
C 4.34313 5.76951 -2.41634  
C 3.11893 1.99069 -3.85896  
C 1.88265 1.89355 -4.51771  
C 1.11478 3.08268 -4.74554  
C 1.72576 4.34791 -4.63482  
C -0.31160 2.98180 -4.80156  
C -1.10041 4.14831 -4.74403  
C -0.44438 5.39222 -4.96783  
C 0.92085 5.48882 -4.91496  
C -0.92067 1.69523 -4.62716  
C -2.20473 1.61512 -4.06457  
C -2.87595 2.82174 -3.67655  
C -2.42528 4.06603 -4.16112  
C -4.04803 5.17720 -2.73103  
C -3.15751 5.22325 -3.77126  
C -2.70283 0.34850 -3.63396  
C -2.05063 -0.83548 -3.03304  
C -0.74497 -0.75371 -4.60457  
C -0.13732 0.50917 -4.75653  
C 1.28569 0.60984 -4.70045  
C 2.05092 -0.55555 -4.49571  
C 3.30810 -0.45679 -3.82598  
C 3.75512 0.80466 -3.38408  
C 4.59606 0.88264 -2.23292  
C 4.96036 -0.30312 -1.56424  
C 5.21977 -0.26085 -0.16086  
C 5.10565 0.96519 0.52456  
C 4.73414 0.96173 1.90314  
C 4.48894 -0.26734 2.54770  
C 3.55903 -0.31489 3.62988  
C 2.90702 0.86871 4.02997  
C 1.60274 0.78697 4.60488  
C 0.99532 -0.47580 4.75756  
C -0.42781 -0.57634 4.70704  
C -1.19335 0.58936 4.50468  
C -2.45185 0.49098 3.83753  
C -2.89853 -0.77003 3.39351  
C -3.73653 -0.84710 2.24014  
C -4.08987 0.33908 1.56724  
C -2.52634 -2.09997 -3.57139  
C -1.87932 -3.30861 -3.99070  
C -0.57080 -3.22660 -4.56514  
C 0.04549 -1.93871 -4.69792  
C 1.44487 -1.83945 -4.64359  
C 2.22423 -3.02830 -4.45725  
C 3.48455 -2.92914 -3.78592  
C 3.92098 -1.64403 -3.32395  
C 4.74845 -1.56713 -2.19218  
C 5.13768 -2.77518 -1.52534  
C 5.39795 -2.73270 -0.11845



|   |          |          |          |
|---|----------|----------|----------|
| C | 5.25981  | -1.48432 | 0.57288  |
| C | 4.89424  | -1.48777 | 1.92857  |
| C | 4.66643  | -2.73945 | 2.58950  |
| C | 3.73379  | -2.78715 | 3.67405  |
| C | 3.06158  | -1.58134 | 4.06098  |
| C | 1.77842  | -1.66180 | 4.62570  |
| C | 1.16984  | -2.94833 | 4.80099  |
| C | -0.25674 | -3.04922 | 4.74871  |
| C | -1.02525 | -1.85994 | 4.52434  |
| C | -2.26280 | -1.95662 | 3.86770  |
| C | -2.72780 | -3.24263 | 3.43622  |
| C | -3.57081 | -3.31961 | 2.28169  |
| C | -3.91548 | -2.10810 | 1.59650  |
| C | -2.39401 | -4.55831 | -3.59187 |
| C | -1.73284 | -5.72212 | -4.07780 |
| C | -0.48109 | -5.64397 | -4.62773 |
| C | 0.19775  | -4.39592 | -4.73014 |
| C | 1.64239  | -4.29344 | -4.67419 |
| C | 2.47968  | -5.43395 | -4.51414 |
| C | 3.68532  | -5.33902 | -3.87106 |
| C | 4.13916  | -4.09619 | -3.34418 |
| C | 4.99407  | -4.01677 | -2.17621 |
| C | 5.43932  | -5.17551 | -1.47815 |
| C | 5.68898  | -5.13479 | -0.13194 |
| C | 5.51048  | -3.93304 | 0.61080  |
| C | 5.13208  | -3.93681 | 2.01014  |
| C | 4.91081  | -5.14257 | 2.73429  |
| C | 4.01810  | -5.18831 | 3.77210  |
| C | 3.28327  | -4.03139 | 4.15863  |
| C | 1.95882  | -4.11464 | 4.74159  |
| C | 1.30339  | -5.35900 | 4.96504  |
| C | -0.06188 | -5.45557 | 4.91450  |
| C | -0.86774 | -4.31443 | 4.63759  |
| C | -2.14550 | -4.41415 | 3.96005  |
| C | -2.67997 | -5.66041 | 3.52470  |
| C | -3.48708 | -5.73414 | 2.42090  |
| C | -3.81530 | -4.56707 | 1.67336  |
| H | 3.03192  | 6.73397  | 3.92912  |
| H | 0.83021  | 6.59640  | 4.89464  |
| H | -1.26145 | 6.45009  | 4.80855  |
| H | -3.38036 | 6.28334  | 3.67538  |
| H | -4.63629 | 6.16363  | 1.99207  |
| H | -5.07450 | 6.08982  | -0.37564 |
| H | -4.50172 | 6.10280  | -2.39517 |
| H | -2.93817 | 6.18335  | -4.22426 |
| H | -1.02511 | 6.30143  | -5.07521 |
| H | 1.37468  | 6.47083  | -4.98457 |
| H | 3.22324  | 6.61638  | -3.99744 |
| H | 4.64237  | 6.74730  | -2.05649 |
| H | 5.01506  | 6.80998  | 0.00672  |
| H | 4.38876  | 6.80435  | 2.32977  |
| H | -2.36672 | -6.58257 | 4.00090  |
| H | -3.78613 | -6.71167 | 2.06011  |
| H | -4.16581 | -6.77282 | -0.00308 |
| H | -3.53632 | -6.76985 | -2.32553 |
| H | -2.17076 | -6.70138 | -3.92129 |
| H | 0.03111  | -6.56364 | -4.88653 |
| H | 2.12289  | -6.41508 | -4.80577 |
| H | 4.24183  | -6.24796 | -3.67282 |
| H | 5.48311  | -6.13243 | -1.98586 |
| H | 5.92200  | -6.06083 | 0.38122  |
| H | 5.36831  | -6.06742 | 2.40178  |
| H | 3.80010  | -6.14772 | 4.22717  |
| H | 1.88434  | -6.26831 | 5.07020  |
| H | -0.51548 | -6.43774 | 4.98356  |
| C | -7.61108 | 1.30687  | -0.55888 |
| C | -7.54495 | 0.06727  | -1.18613 |
| C | -7.43248 | -1.11124 | -0.43961 |
| C | -7.38637 | -1.01546 | 0.95209  |
| C | -7.44623 | 0.22611  | 1.58552  |
| C | -7.55865 | 1.39150  | 0.83252  |
| H | -7.56546 | 0.00802  | -2.27198 |
| C | -7.33330 | -2.44321 | -1.13722 |
| H | -7.28590 | -1.92137 | 1.54513  |
| H | -7.39226 | 0.28121  | 2.66888  |

|   |          |          |          |
|---|----------|----------|----------|
| H | -7.59102 | 2.36019  | 1.32250  |
| H | -7.11456 | -3.24717 | -0.43009 |
| H | -8.26490 | -2.68796 | -1.65742 |
| H | -6.53493 | -2.42628 | -1.88790 |
| H | -7.67765 | 2.21259  | -1.15528 |

# Benzene-concave surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -0.15232 | 1.14476  | -0.91347 |
| C | 1.24187  | 1.13815  | -0.87965 |
| C | 1.93203  | -0.07079 | -0.82508 |
| C | 1.22757  | -1.27144 | -0.77506 |
| C | -0.16653 | -1.26500 | -0.81086 |
| C | -0.85616 | -0.05747 | -0.89458 |
| H | -1.94188 | -0.05284 | -0.93442 |
| C | -0.59509 | -3.23044 | -3.47530 |
| C | -1.83669 | -3.73059 | -2.98079 |
| C | -3.07372 | -3.22531 | -3.50160 |
| C | -3.06467 | -2.00005 | -4.24040 |
| C | -1.81894 | -1.31557 | -4.42472 |
| C | -0.58756 | -1.99681 | -4.19392 |
| C | -4.27847 | -1.35200 | -4.54399 |
| C | -4.27800 | 0.08663  | -4.72224 |
| C | -3.06372 | 0.78839  | -4.58265 |
| C | -1.81870 | 0.07842  | -4.59393 |
| C | -0.58713 | 0.79443  | -4.53070 |
| C | -0.59450 | 2.16639  | -4.13864 |
| C | -1.83582 | 2.77915  | -3.79525 |
| C | -3.07276 | 2.15901  | -4.17267 |
| C | -4.29604 | 2.80160  | -3.89624 |
| C | -4.31135 | 3.87828  | -2.92581 |
| C | -3.10187 | 4.24697  | -2.30502 |
| C | -1.84978 | 3.83453  | -2.86953 |
| C | -0.62119 | 4.27731  | -2.29164 |
| C | -0.63617 | 4.78732  | -0.95605 |
| C | -1.87804 | 4.84564  | -0.25305 |
| C | -3.11629 | 4.76504  | -0.97191 |
| C | 0.57648  | 4.87703  | -0.24211 |
| C | 0.56356  | 4.71168  | 1.17686  |
| C | -0.66064 | 4.47197  | 1.83247  |
| C | -1.89033 | 4.68927  | 1.14266  |
| C | 1.81992  | 4.77659  | -0.93770 |
| C | 3.05542  | 4.88359  | -0.21692 |
| C | 3.04158  | 4.72395  | 1.20590  |
| C | 1.79278  | 4.45988  | 1.85714  |
| C | 4.28101  | 4.84571  | -0.91067 |
| C | 5.47152  | 5.00885  | -0.14552 |
| C | 5.45718  | 4.86356  | 1.21580  |
| C | 4.25206  | 4.54395  | 1.90411  |
| C | 1.78436  | 3.70659  | 3.04258  |
| C | 3.02373  | 3.21791  | 3.57209  |
| C | 4.24362  | 3.76367  | 3.12537  |
| C | 1.83459  | 4.27351  | -2.24961 |
| C | 3.08562  | 3.87082  | -2.82435 |
| C | 4.29710  | 4.31751  | -2.25943 |
| C | 0.54608  | 3.20841  | 3.54693  |
| C | -0.66975 | 3.70780  | 3.03883  |
| C | 0.60558  | 3.87376  | -2.85835 |
| C | -1.90796 | 3.18828  | 3.52210  |
| C | -3.14774 | 3.70778  | 3.02433  |
| C | -3.13878 | 4.47101  | 1.81352  |
| C | -4.35127 | 4.75393  | 1.15452  |
| C | -4.33973 | 4.90371  | -0.28729 |
| C | -4.36874 | 3.24437  | 3.55400  |
| C | -5.56433 | 3.82899  | 3.04734  |
| C | -5.55594 | 4.55798  | 1.88779  |
| C | -5.51863 | 4.35627  | -2.34050 |
| C | -5.53248 | 4.85260  | -1.06435 |
| C | 0.61869  | 2.79472  | -3.79407 |
| C | -5.47790 | 0.85218  | -4.74185 |
| C | -5.48706 | 2.16220  | -4.34211 |
| C | 0.63298  | 0.09260  | -4.56117 |
| C | 0.63273  | -1.32336 | -4.39389 |
| C | -4.29697 | -3.77121 | -3.06440 |
| C | -5.48842 | -3.26569 | -3.65759 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.47882 | -2.09772 | -4.37332 |
| C | -1.85051 | -4.49497 | -1.80222 |
| C | -3.10193 | -4.73378 | -1.14398 |
| C | -4.31151 | -4.54900 | -1.84137 |
| C | 0.61835  | -3.74897 | -2.97919 |
| C | 0.60515  | -4.53077 | -1.78229 |
| C | -0.62158 | -4.75716 | -1.12358 |
| C | -0.63638 | -4.87152 | 0.30171  |
| C | -1.87803 | -4.73443 | 0.99352  |
| C | -3.11632 | -4.85994 | 0.28158  |
| C | -4.33970 | -4.80419 | 0.97807  |
| C | -5.53228 | -4.97095 | 0.21712  |
| C | -5.51861 | -4.84623 | -1.14646 |
| C | -1.88997 | -4.20414 | 2.29323  |
| C | -3.13839 | -3.81543 | 2.88193  |
| C | -4.35115 | -4.26683 | 2.32414  |
| C | 0.57622  | -4.75901 | 1.01150  |
| C | 0.56392  | -4.21440 | 2.33113  |
| C | -0.66022 | -3.80884 | 2.89882  |
| C | -0.66923 | -2.75657 | 3.86321  |
| C | -1.90767 | -2.13133 | 4.19695  |
| C | -3.14751 | -2.76169 | 3.85006  |
| C | -4.36866 | -2.17934 | 4.24484  |
| C | -5.56380 | -2.87554 | 3.90711  |
| C | -5.55543 | -3.88379 | 2.97990  |
| C | -1.91256 | -0.79370 | 4.62276  |
| C | -3.15720 | -0.08645 | 4.70066  |
| C | -4.37374 | -0.79759 | 4.68341  |
| C | 0.54667  | -2.14438 | 4.22666  |
| C | 0.54214  | -0.78424 | 4.65832  |
| C | -0.67867 | -0.08255 | 4.71347  |
| C | -0.67873 | 1.33365  | 4.53451  |
| C | -1.91257 | 1.99937  | 4.26966  |
| C | -3.15701 | 1.33369  | 4.52109  |
| C | -4.37347 | 2.01790  | 4.32693  |
| C | -5.57383 | 1.31716  | 4.63488  |
| C | -5.57400 | -0.04180 | 4.80753  |
| C | 0.54185  | 1.99979  | 4.30646  |
| C | 3.01999  | 2.00407  | 4.33059  |
| C | 1.77623  | 1.32283  | 4.53925  |
| C | 1.77646  | -0.07029 | 4.71534  |
| C | 3.02051  | -0.78190 | 4.68228  |
| C | 3.02485  | -2.14705 | 4.25300  |
| C | 1.78512  | -2.75413 | 3.86581  |
| C | 1.79342  | -3.79077 | 2.91912  |
| C | 3.04176  | -4.22130 | 2.36235  |
| C | 3.05442  | -4.76330 | 1.03809  |
| C | 1.81903  | -4.85775 | 0.31581  |
| C | 1.83393  | -4.74468 | -1.08503 |
| C | 3.08543  | -4.51992 | -1.74915 |
| C | 3.09720  | -3.73706 | -2.94811 |
| C | 1.85798  | -3.21102 | -3.44014 |
| C | 1.86456  | -1.99574 | -4.14401 |
| C | 3.10774  | -1.32316 | -4.37848 |
| C | 3.10803  | 0.09740  | -4.55120 |
| C | 1.86477  | 0.80610  | -4.48288 |
| C | 1.85786  | 2.15676  | -4.10044 |
| C | 3.09725  | 2.79374  | -3.76665 |
| C | 5.43899  | 3.26393  | 3.71643  |
| C | 5.43512  | 2.10158  | 4.44109  |
| C | 4.23595  | 1.35757  | 4.62863  |
| C | 4.23640  | -0.08086 | 4.81026  |
| C | 5.43616  | -0.84750 | 4.81193  |
| C | 5.44020  | -2.15452 | 4.40273  |
| C | 4.24475  | -2.78914 | 3.96069  |
| C | 4.25284  | -3.86298 | 2.98707  |
| C | 5.45695  | -4.36011 | 2.41136  |
| C | 5.47011  | -4.87286 | 1.14182  |
| C | 4.27951  | -4.92481 | 0.36133  |
| C | 4.29599  | -4.79224 | -1.08148 |
| C | 5.50435  | -4.58787 | -1.80692 |
| C | 5.51543  | -3.84441 | -2.95652 |
| C | 4.31971  | -3.25438 | -3.45727 |
| C | 4.32500  | -2.01070 | -4.20069 |
| C | 5.52515  | -1.30739 | -4.50200 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.52520  | 0.05214  | -4.66995 |
| C | 4.32518  | 0.80785  | -4.54707 |
| C | 4.31953  | 2.19786  | -4.13806 |
| C | 5.51499  | 2.89911  | -3.81151 |
| C | 5.50473  | 3.92331  | -2.90272 |
| H | 3.01813  | -0.07650 | -0.80919 |
| H | 1.76771  | -2.21091 | -0.70377 |
| H | -0.71873 | -2.19939 | -0.76968 |
| H | -0.69299 | 2.08616  | -0.95363 |
| H | 1.79340  | 2.07408  | -0.89323 |
| H | -6.43985 | -3.74582 | -3.45886 |
| H | -6.42293 | -1.69448 | -4.72128 |
| H | -6.42251 | 0.37448  | -4.97591 |
| H | -6.43876 | 2.67641  | -4.27182 |
| H | -6.46263 | 4.22957  | -2.85808 |
| H | -6.48641 | 5.10014  | -0.61254 |
| H | -6.50162 | 4.89453  | 1.47840  |
| H | -6.51665 | 3.61218  | 3.51776  |
| H | -6.52315 | 1.84064  | 4.63347  |
| H | -6.52398 | -0.54714 | 4.93852  |
| H | -6.51643 | -2.54258 | 4.30303  |
| H | -6.50157 | -4.31503 | 2.67307  |
| H | -6.48654 | -5.08602 | 0.71829  |
| H | -6.46202 | -4.86487 | -1.68028 |
| H | 6.46851  | 2.55634  | -4.19667 |
| H | 6.45015  | 4.35585  | -2.59558 |
| H | 6.42510  | 5.13989  | -0.64407 |
| H | 6.39933  | 4.88582  | 1.75165  |
| H | 6.38886  | 3.74320  | 3.50855  |
| H | 6.38188  | 1.70099  | 4.78494  |
| H | 6.38357  | -0.37177 | 5.03856  |
| H | 6.39104  | -2.66832 | 4.31972  |
| H | 6.39997  | -4.24027 | 2.93234  |
| H | 6.42269  | -5.13827 | 0.69732  |
| H | 6.44909  | -4.92361 | -1.39472 |
| H | 6.46902  | -3.61665 | -3.41904 |
| H | 6.47424  | -1.83128 | -4.50638 |
| H | 6.47491  | 0.55735  | -4.80339 |

#### Benzene-graphene, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -2.71374 | -0.91935 | 2.89053  |
| C | -1.73739 | -1.91256 | 2.87277  |
| C | -0.38682 | -1.56300 | 2.88322  |
| C | -0.01467 | -0.22105 | 2.90637  |
| C | -0.99313 | 0.77313  | 2.92287  |
| C | -2.34195 | 0.42504  | 2.91502  |
| H | -0.70193 | 1.81996  | 2.92311  |
| C | -0.61059 | -1.64376 | -0.35075 |
| C | 0.82319  | -1.65274 | -0.30572 |
| C | 1.53292  | -2.89360 | -0.29139 |
| C | 0.82043  | -4.12031 | -0.30954 |
| C | -0.63730 | -4.11063 | -0.31426 |
| C | -1.33413 | -2.87575 | -0.34891 |
| C | 1.53635  | -0.43691 | -0.27602 |
| C | 2.96922  | -0.44691 | -0.22903 |
| C | 3.67211  | -1.66769 | -0.22606 |
| C | 2.96068  | -2.90368 | -0.25768 |
| C | 3.68183  | 0.79044  | -0.19413 |
| C | 5.11404  | 0.77997  | -0.15610 |
| C | 5.81628  | -0.45449 | -0.15461 |
| C | 5.10993  | -1.67605 | -0.18815 |
| C | 7.25331  | -0.45349 | -0.11734 |
| C | 7.94480  | 0.78541  | -0.08432 |
| C | 7.27089  | 1.98451  | -0.08678 |
| C | 5.83080  | 1.99384  | -0.12303 |
| C | 2.98424  | 2.01433  | -0.19359 |
| C | 3.70814  | 3.24663  | -0.15837 |
| C | 5.13254  | 3.22951  | -0.12481 |
| C | 5.82356  | -2.90200 | -0.18446 |
| C | 7.25536  | -2.88949 | -0.14607 |
| C | 7.93771  | -1.66562 | -0.11418 |
| C | 5.86104  | 4.44965  | -0.09351 |
| C | 7.30177  | 4.41706  | -0.05765 |
| C | 7.97407  | 3.24526  | -0.05385 |
| C | 3.66624  | -4.13841 | -0.25794 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.13118  | -4.14915 | -0.21693 |
| C | 5.87142  | -5.32445 | -0.20599 |
| C | 7.27810  | -5.30903 | -0.16881 |
| C | 7.96211  | -4.12075 | -0.14032 |
| C | 1.54595  | -5.31319 | -0.32584 |
| C | 2.92867  | -5.32105 | -0.30165 |
| C | 1.55104  | 2.02382  | -0.23462 |
| C | 0.83642  | 0.80733  | -0.27678 |
| C | -1.30866 | -0.41945 | -0.34366 |
| C | -0.59435 | 0.81577  | -0.32093 |
| C | -2.74113 | -0.41164 | -0.36460 |
| C | -3.45807 | -1.62364 | -0.36612 |
| C | -2.76177 | -2.86791 | -0.36042 |
| C | -3.48245 | -4.09380 | -0.34070 |
| C | -2.76001 | -5.28510 | -0.28256 |
| C | -1.37713 | -5.29409 | -0.26863 |
| C | 3.02380  | 4.48825  | -0.15699 |
| C | 1.56629  | 4.49466  | -0.18314 |
| C | 0.84984  | 3.26784  | -0.22339 |
| C | -0.57831 | 3.27619  | -0.25235 |
| C | -1.29392 | 2.04095  | -0.29550 |
| C | -2.72691 | 2.04860  | -0.30520 |
| C | -3.43863 | 0.83311  | -0.33161 |
| C | -4.87131 | 0.84046  | -0.32359 |
| C | -5.58867 | -0.38521 | -0.33676 |
| C | -4.89632 | -1.61495 | -0.35592 |
| C | -5.62525 | -2.83191 | -0.36255 |
| C | -4.94756 | -4.08727 | -0.36829 |
| C | -7.02593 | -0.36682 | -0.33251 |
| C | -7.72528 | -1.57042 | -0.35092 |
| C | -7.05720 | -2.80231 | -0.36706 |
| C | -7.77868 | -4.02494 | -0.38907 |
| C | -7.10851 | -5.22126 | -0.40873 |
| C | -5.70162 | -5.25343 | -0.39924 |
| C | -7.70312 | 0.88003  | -0.31163 |
| C | -7.01476 | 2.07084  | -0.29349 |
| C | -5.57421 | 2.06252  | -0.29749 |
| C | -4.86136 | 3.28984  | -0.27624 |
| C | -3.43650 | 3.28941  | -0.27443 |
| C | -2.73782 | 4.52266  | -0.24590 |
| C | -1.28034 | 4.51181  | -0.22964 |
| C | -0.54051 | 5.69651  | -0.18624 |
| C | 0.84005  | 5.68825  | -0.16516 |
| C | -5.57571 | 4.51835  | -0.25381 |
| C | -7.01717 | 4.50325  | -0.25232 |
| C | -7.70340 | 3.33976  | -0.27054 |
| C | -4.85863 | 5.71559  | -0.23352 |
| C | -3.47446 | 5.71622  | -0.22952 |
| C | 5.15822  | 5.65531  | -0.09855 |
| C | 3.77436  | 5.67286  | -0.12960 |
| H | -7.53820 | 5.45609  | -0.23484 |
| H | 7.83383  | 5.36360  | -0.03287 |
| H | -8.81199 | -1.55612 | -0.35211 |
| H | -8.78999 | 0.88440  | -0.30897 |
| H | -8.78926 | 3.33147  | -0.26803 |
| H | -8.86391 | -3.99124 | -0.39323 |
| H | -7.65852 | -6.15605 | -0.43177 |
| H | -5.21795 | -6.22214 | -0.42145 |
| H | -3.27273 | -6.23780 | -0.23813 |
| H | -0.88053 | -6.25401 | -0.21094 |
| H | 1.03757  | -6.26781 | -0.36506 |
| H | 3.42928  | -6.28101 | -0.31836 |
| H | 5.37697  | -6.28769 | -0.22505 |
| H | 7.81702  | -6.25055 | -0.16244 |
| H | 9.04729  | -4.10015 | -0.11173 |
| H | 9.02414  | -1.66468 | -0.08575 |
| H | 9.03129  | 0.77665  | -0.05673 |
| H | 9.05942  | 3.22404  | -0.02618 |
| H | -5.39930 | 6.65728  | -0.21931 |
| H | -2.96767 | 6.67262  | -0.21259 |
| H | -1.03956 | 6.65671  | -0.16496 |
| H | 1.34980  | 6.64236  | -0.12862 |
| H | 3.27910  | 6.63543  | -0.13367 |
| H | 5.70970  | 6.59059  | -0.07721 |
| H | 0.37443  | -2.33783 | 2.84918  |

|   |          |          |         |
|---|----------|----------|---------|
| H | 1.03670  | 0.05223  | 2.89839 |
| H | -3.10376 | 1.19949  | 2.91307 |
| H | -3.76544 | -1.19113 | 2.86583 |
| H | -2.02702 | -2.95904 | 2.83390 |

#### Benzene-convex surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | 7.74075  | 0.16243  | -0.64786 |
| C | 7.80547  | 0.03898  | 0.73919  |
| C | 7.58135  | -1.19770 | 1.34105  |
| C | 7.29418  | -2.31288 | 0.55491  |
| C | 7.22639  | -2.19050 | -0.83142 |
| C | 7.45124  | -0.95236 | -1.43285 |
| H | 7.10666  | -3.27444 | 1.02401  |
| C | 4.07972  | -1.59775 | 0.70969  |
| C | 3.68307  | -1.50853 | 2.07715  |
| C | 3.04518  | -2.63072 | 2.68653  |
| C | 3.13227  | -3.92495 | 2.07601  |
| C | 3.54110  | -4.01660 | 0.70642  |
| C | 3.84490  | -2.80990 | -0.00514 |
| C | 3.37368  | -5.22638 | 0.00323  |
| C | 3.11093  | -6.39730 | 0.77026  |
| C | 2.71837  | -6.30919 | 2.07952  |
| C | 2.56154  | -5.04401 | 2.71436  |
| C | 2.11598  | -2.41937 | 3.71776  |
| C | 1.27323  | -3.50199 | 4.13378  |
| C | 1.59966  | -4.82568 | 3.77694  |
| C | 3.64147  | -2.76164 | -1.39358 |
| C | 3.13023  | -3.91944 | -2.06720 |
| C | 3.16079  | -5.17588 | -1.43017 |
| C | 1.82807  | -1.08577 | 4.13799  |
| C | 2.67138  | -0.02793 | 3.74284  |
| C | 3.61561  | -0.24292 | 2.69334  |
| C | 4.22095  | 0.88569  | 2.06469  |
| C | 4.60916  | 0.79650  | 0.71930  |
| C | 4.40123  | -0.42063 | 0.00777  |
| C | 4.19581  | -0.37174 | -1.40262 |
| C | 3.67924  | -1.50273 | -2.06424 |
| C | 2.36348  | 1.31045  | 4.13173  |
| C | 3.22851  | 2.38823  | 3.74790  |
| C | 4.17472  | 2.17228  | 2.69610  |
| C | 4.83725  | 3.26878  | 2.10936  |
| C | 5.25053  | 3.17274  | 0.72210  |
| C | 4.96478  | 1.99071  | 0.01140  |
| C | 4.76174  | 2.03986  | -1.40385 |
| C | 4.20932  | 0.89286  | -2.06219 |
| C | 2.96230  | 3.69813  | 4.19346  |
| C | 3.87837  | 4.71829  | 3.80982  |
| C | 4.78373  | 4.51112  | 2.80279  |
| C | 4.84026  | 3.27230  | -2.08271 |
| C | 5.44484  | 4.36073  | -1.39132 |
| C | 5.64366  | 4.31197  | -0.03649 |
| C | 3.44433  | 1.07074  | -3.22560 |
| C | 3.23132  | 2.39687  | -3.72642 |
| C | 4.04620  | 3.45756  | -3.28172 |
| C | 2.89870  | -1.32217 | -3.24568 |
| C | 2.67031  | -0.01795 | -3.72814 |
| C | 1.46722  | 0.26056  | -4.44405 |
| C | 1.07493  | 1.61940  | -4.63678 |
| C | 2.02541  | 2.67614  | -4.44463 |
| C | 1.65606  | 4.01107  | -4.70409 |
| C | 2.65589  | 5.01087  | -4.53309 |
| C | 3.81053  | 4.74342  | -3.84659 |
| C | -0.28946 | 1.93464  | -4.74016 |
| C | -0.70014 | 3.30544  | -4.65275 |
| C | 0.24743  | 4.33631  | -4.81206 |
| C | 0.53510  | -0.77580 | -4.65363 |
| C | -0.85220 | -0.45498 | -4.75873 |
| C | -1.25834 | 0.89022  | -4.65173 |
| C | -2.55284 | 1.18865  | -4.12897 |
| C | -2.84025 | 2.52240  | -3.71020 |
| C | -1.99791 | 3.60455  | -4.12868 |
| C | -2.32401 | 4.92875  | -3.77366 |
| C | -1.47196 | 5.96289  | -4.25556 |
| C | -0.23004 | 5.67675  | -4.75739 |

C -3.77044 2.73527 -2.67995  
 C -3.85555 4.03026 -2.07060  
 C -3.28403 5.14838 -2.70978  
 C -3.39639 0.13150 -3.73247  
 C -4.34275 0.34804 -2.68532  
 C -4.41143 1.61466 -2.07139  
 C -4.81926 1.70769 -0.70605  
 C -4.57379 2.91787 0.00954  
 C -4.26407 4.12347 -0.70175  
 C -4.09364 5.33238 0.00165  
 C -3.82861 6.50273 -0.76510  
 C -3.43785 6.41373 -2.07486  
 C -4.36783 2.86782 1.39761  
 C -3.85338 4.02412 2.07124  
 C -3.88236 5.28096 1.43511  
 C -5.14372 0.53014 -0.00309  
 C -4.93420 0.84927 1.40830  
 C -4.40732 1.60808 2.06698  
 C -3.62462 1.42574 3.24696  
 C -2.82567 2.50843 3.72243  
 C -3.06919 3.84146 3.25439  
 C -2.32838 4.91896 3.77944  
 C -2.64726 6.22333 3.30554  
 C -3.39769 6.39815 2.17312  
 C -1.64337 2.23427 4.42826  
 C -0.70632 3.29388 4.66290  
 C -1.10726 4.63580 4.50761  
 C -3.39520 0.12062 3.72617  
 C -2.19299 -0.15834 4.44360  
 C -1.26137 0.87788 4.65572  
 C 0.12578 0.55734 4.76502  
 C 1.08928 1.60324 4.64330  
 C 0.68416 2.97253 4.77219  
 C 1.64725 3.99965 4.72413  
 C 1.18770 5.33540 4.90139  
 C -0.14283 5.64313 4.79608  
 C 0.53234 -0.78779 4.65760  
 C -0.02567 -3.20328 4.65550  
 C -0.43664 -1.83247 4.74294  
 C -1.80071 -1.51715 4.63618  
 C -2.75092 -2.57352 4.44291  
 C -3.95671 -2.29377 3.72473  
 C -4.17099 -0.96739 3.22472  
 C -4.94110 -0.78797 2.06471  
 C -5.49594 -1.93494 1.40752  
 C -5.70599 -1.88384 -0.00742  
 C -5.35454 -0.68811 -0.71597  
 C -4.95348 -0.77963 -2.05873  
 C -4.90428 -2.06641 -2.68903  
 C -3.95537 -2.28352 -3.73851  
 C -3.08931 -1.20689 -4.12146  
 C -1.81581 -1.50053 -4.63445  
 C -1.41125 -2.86992 -4.76301  
 C -0.02061 -3.19165 -4.65581  
 C 0.91713 -2.13208 -4.42469  
 C 2.10032 -2.40574 -3.72008  
 C 2.34424 -3.73811 -3.24983  
 C 0.74623 -5.86033 4.25564  
 C -0.49638 -5.57476 4.75605  
 C -0.97360 -4.23418 4.81210  
 C -2.38194 -3.90851 4.70273  
 C -3.38231 -4.90786 4.53268  
 C -4.53721 -4.64004 3.84702  
 C -4.77232 -3.35422 3.28172  
 C -5.56802 -3.16872 2.08428  
 C -6.16872 -4.25934 1.39287  
 C -6.36928 -4.21063 0.03889  
 C -5.98372 -3.06813 -0.71868  
 C -5.56837 -3.16309 -2.10424  
 C -5.51559 -4.40524 -2.79861  
 C -4.60819 -4.61280 -3.80318  
 C -3.68953 -3.59356 -4.18363  
 C -2.37475 -3.89657 -4.71326  
 C -1.91591 -5.23291 -4.88871  
 C -0.58543 -5.54089 -4.78404

C 0.38005 -4.53351 -4.49869  
 C 1.60252 -4.81619 -3.77255  
 C 1.92246 -6.12018 -3.29795  
 C 2.67516 -6.29380 -2.16685  
 H -1.75537 7.00185 -4.13146  
 H 0.42787 6.49910 -5.01421  
 H 2.46592 6.02931 -4.85236  
 H 4.49591 5.55901 -3.64630  
 H 5.65922 5.28582 -1.91427  
 H 6.00896 5.19996 0.46706  
 H 5.38703 5.34741 2.46818  
 H 3.79514 5.71117 4.23698  
 H 1.90031 6.14406 5.01586  
 H -0.43923 6.68540 4.82896  
 H -2.20826 7.09528 3.77690  
 H -3.52770 7.40222 1.78567  
 H -3.82969 7.47634 -0.28834  
 H -3.14175 7.31964 -2.59147  
 H 1.48290 -6.99268 -3.76781  
 H 2.80612 -7.29762 -1.77901  
 H 3.11505 -7.37106 0.29374  
 H 2.42389 -7.21576 2.59596  
 H 1.02933 -6.89920 4.12989  
 H -1.15496 -6.39739 5.01022  
 H -3.19306 -5.92607 4.85308  
 H -5.22380 -5.45501 3.64867  
 H -6.37753 -5.18598 1.91515  
 H -6.72901 -5.10033 -0.46543  
 H -6.12204 -5.24031 -2.46696  
 H -4.52613 -5.60506 -4.23200  
 H -2.62882 -6.04156 -5.00117  
 H -0.28954 -6.58336 -4.81531  
 H 7.62349 -1.29152 2.42199  
 H 6.98622 -3.05616 -1.44158  
 H 7.38765 -0.85394 -2.51252  
 H 7.90101 1.13021 -1.11454  
 H 8.01630 0.91143 1.35106

# Ethane-concave surface of SWCNT, CPCM

C -4.28888 2.55495 4.10224  
 C -4.27929 3.67945 3.18769  
 C -3.05835 4.06305 2.59861  
 C -1.81917 3.59782 3.14925  
 C -1.82847 2.50940 4.03568  
 C -3.07664 1.88791 4.36901  
 C -5.47344 4.20901 2.62042  
 C -5.46715 4.78867 1.37963  
 C -4.26608 4.87795 0.61912  
 C -3.05161 4.66911 1.30222  
 C -1.80580 4.78789 0.60241  
 C -1.80311 4.75936 -0.80123  
 C -3.04633 4.61173 -1.50014  
 C -4.26346 4.84685 -0.83029  
 C -0.57262 4.64925 1.30777  
 C -0.57947 4.04427 2.60078  
 C -3.04799 3.95393 -2.77120  
 C -4.26660 3.54538 -3.34852  
 C -5.46341 4.09470 -2.80639  
 C -5.46194 4.72344 -1.58962  
 C -1.80663 3.46708 -3.29787  
 C -0.56909 3.93603 -2.76328  
 C -0.56718 4.59262 -1.49550  
 C 0.65202 4.75876 -0.80837  
 C 0.64925 4.78791 0.61927  
 C -4.27241 2.38423 -4.21608  
 C -3.05920 1.70691 -4.45001  
 C -1.81241 2.34199 -4.13785  
 C -0.58083 1.68775 -4.44019  
 C 0.64243 2.32490 -4.15156  
 C 0.64844 3.46937 -3.29831  
 C 1.88584 3.91043 -2.74039  
 C 1.88768 4.55582 -1.49340  
 C 1.88214 4.61275 1.31697  
 C 3.12838 4.77276 0.62627

C 3.13118 4.74336 -0.80484  
 C 4.34901 4.61238 -1.50138  
 C 4.34703 3.94666 -2.78906  
 C 3.12711 3.45530 -3.29523  
 C 3.12103 2.30887 -4.15195  
 C 1.87369 1.65660 -4.42332  
 C 4.33449 1.67677 -4.48861  
 C 5.53777 2.39353 -4.23181  
 C 5.54402 3.48943 -3.41037  
 C 4.34345 4.67027 1.33245  
 C 5.54542 4.87988 0.59797  
 C 5.54812 4.85167 -0.77131  
 C 4.33642 4.05710 2.64588  
 C 3.11452 3.58669 3.16683  
 C 1.87541 4.01804 2.58867  
 C 0.63582 3.60050 3.15953  
 C 4.32532 0.25526 -4.77343  
 C 3.10299 -0.44240 -4.70319  
 C 1.86469 0.27971 -4.69783  
 C 0.62464 -0.42615 -4.70054  
 C -0.58996 0.28779 -4.71860  
 C -1.83001 -0.41750 -4.68765  
 C -3.06837 0.30330 -4.73001  
 C -4.29034 -0.39706 -4.77353  
 C -5.48407 0.37500 -4.58425  
 C -5.47523 1.71796 -4.58540  
 C 0.61433 -1.81263 -4.36042  
 C -0.60978 -2.43722 -4.04864  
 C -1.83988 -1.78076 -4.35269  
 C -3.08803 -2.42180 -4.06032  
 C -4.30025 -1.80509 -4.42901  
 C 0.62631 2.49361 4.06074  
 C -0.59811 1.86869 4.37052  
 C 1.84471 -2.45273 -4.02524  
 C 3.09266 -1.83218 -4.36172  
 C 3.10499 2.47768 4.07118  
 C 1.85653 1.83727 4.36503  
 C 4.30503 -2.49959 -4.09690  
 C 5.50899 -1.84999 -4.49135  
 C 5.51898 -0.51983 -4.81724  
 C 4.31717 1.86028 4.43870  
 C 5.52150 2.56576 4.15680  
 C 5.53096 3.62646 3.29030  
 C -0.60846 0.48127 4.70603  
 C 0.60627 -0.23246 4.72217  
 C 1.84641 0.47290 4.69594  
 C 3.08473 -0.24824 4.73551  
 C 4.30684 0.45173 4.78150  
 C -3.08693 0.49702 4.70624  
 C -1.84844 -0.22475 4.69892  
 C -1.85698 -1.60078 4.41984  
 C -0.62545 -2.26855 4.14750  
 C 0.59738 -1.63114 4.43754  
 C 1.82911 -2.28413 4.13374  
 C 3.07568 -1.65062 4.44964  
 C 4.28888 -2.32776 4.21511  
 C 5.49152 -1.66295 4.58750  
 C 5.50038 -0.32079 4.86038  
 C -0.63116 -3.41364 3.29460  
 C 0.58641 -3.87772 2.75808  
 C 1.82363 -3.40810 3.29244  
 C 3.06513 -3.89637 2.76807  
 C 4.28340 -3.48807 3.34645  
 C -5.49324 1.90422 4.49385  
 C -5.50317 0.57351 4.81731  
 C -4.30914 -0.20110 4.77296  
 C -4.31766 -1.62184 4.48502  
 C -3.10395 -2.25278 4.14684  
 C -3.10935 -3.40038 3.29169  
 C -1.86822 -3.85748 2.73841  
 C -1.86995 -4.50809 1.49414  
 C -0.63460 -4.71288 0.80873  
 C 0.58468 -4.54243 1.49475  
 C 1.82091 -4.71285 0.80166  
 C 3.06399 -4.55926 1.49997

|   |          |          |          |
|---|----------|----------|----------|
| C | 4.28153  | -4.79588 | 0.83158  |
| C | 5.47960  | -4.67025 | 1.59097  |
| C | 5.48036  | -4.03884 | 2.80642  |
| C | -0.63154 | -4.74823 | -0.61890 |
| C | 0.59022  | -4.60932 | -1.30794 |
| C | 1.82350  | -4.74583 | -0.60224 |
| C | 3.06963  | -4.62105 | -1.30069 |
| C | 4.28437  | -4.82844 | -0.61775 |
| C | -5.52063 | -2.33927 | 4.22912  |
| C | -5.52654 | -3.43582 | 3.40867  |
| C | -4.32955 | -3.89312 | 2.78755  |
| C | -4.33161 | -4.56225 | 1.50218  |
| C | -3.11355 | -4.69603 | 0.80622  |
| C | -3.11106 | -4.72843 | -0.62486 |
| C | -1.86474 | -4.57233 | -1.31646 |
| C | -1.85829 | -3.96873 | -2.58402 |
| C | -0.61864 | -3.62481 | -3.15237 |
| C | 0.59670  | -3.99591 | -2.59704 |
| C | 1.83568  | -3.54421 | -3.14237 |
| C | 3.07574  | -4.01028 | -2.59442 |
| C | 4.29619  | -3.62485 | -3.18330 |
| C | 5.49087  | -4.15467 | -2.61766 |
| C | 5.48538  | -4.73638 | -1.37781 |
| C | -5.53095 | -4.80283 | 0.77311  |
| C | -5.52856 | -4.83199 | -0.59605 |
| C | -4.32651 | -4.62292 | -1.33033 |
| C | -4.31940 | -4.00643 | -2.64175 |
| C | -3.09721 | -3.53398 | -3.16002 |
| C | -5.51378 | -3.57465 | -3.28566 |
| C | -5.50434 | -2.51190 | -4.14960 |
| C | 0.30865  | -1.27751 | -0.30666 |
| C | -1.12872 | -1.26275 | 0.20804  |
| H | -1.15902 | -1.31624 | 1.30251  |
| H | 6.43675  | -2.19269 | 4.55446  |
| H | 6.45283  | 0.16685  | 5.03403  |
| H | 6.46684  | 2.20236  | 4.54334  |
| H | 6.48360  | 4.06737  | 3.01952  |
| H | 6.49390  | 4.95629  | 1.11736  |
| H | 6.49863  | 4.90646  | -1.28977 |
| H | 6.49556  | 3.94179  | -3.15507 |
| H | 6.48449  | 2.01486  | -4.59981 |
| H | 6.47202  | -0.03919 | -5.00678 |
| H | 6.45424  | -2.37764 | -4.43448 |
| H | 6.44154  | -4.00640 | -3.11700 |
| H | 6.43143  | -5.02917 | -0.93659 |
| H | 6.42772  | -4.97801 | 1.16488  |
| H | 6.42914  | -3.86838 | 3.30230  |
| H | -6.42435 | 4.06261  | 3.11987  |
| H | -6.41284 | 5.08235  | 0.93823  |
| H | -6.40986 | 5.03031  | -1.16242 |
| H | -6.41251 | 3.92487  | -3.30189 |
| H | -6.42054 | 2.24761  | -4.55301 |
| H | -6.43657 | -0.11325 | -5.02590 |
| H | -6.44952 | -2.14862 | -4.53663 |
| H | -6.46626 | -4.01710 | -3.01685 |
| H | -6.47708 | -4.90770 | -1.11544 |
| H | -6.48129 | -4.85659 | 1.29195  |
| H | -6.47783 | -3.88931 | 3.15449  |
| H | -6.46731 | -1.96117 | 4.59780  |
| H | -6.45629 | 0.09217  | 5.00460  |
| H | -6.43864 | 2.43154  | 4.43617  |
| H | -1.64762 | -0.34877 | -0.09542 |
| H | -1.70072 | -2.11240 | -0.17960 |
| H | 0.34044  | -1.27633 | -1.40266 |
| H | 0.86109  | -0.40042 | 0.04313  |
| H | 0.84613  | -2.16720 | 0.03849  |

#### Ethane-graphene, CPCM

|   |         |         |          |
|---|---------|---------|----------|
| C | 7.18969 | 4.44806 | -0.06678 |
| C | 5.74843 | 4.47604 | -0.07220 |
| C | 5.02322 | 3.25367 | -0.08310 |
| C | 5.72519 | 2.02007 | -0.08930 |
| C | 7.16569 | 2.01545 | -0.08218 |
| C | 7.86557 | 3.27835 | -0.07102 |
| C | 5.01176 | 0.80386 | -0.10163 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.71749  | -0.42846 | -0.10608 |
| C | 7.15480  | -0.42271 | -0.09668 |
| C | 7.84309  | 0.81827  | -0.08555 |
| C | 5.01473  | -1.65241 | -0.11877 |
| C | 3.57658  | -1.64889 | -0.13049 |
| C | 2.87048  | -0.42996 | -0.12585 |
| C | 3.57922  | 0.80987  | -0.10978 |
| C | 2.87822  | 2.03176  | -0.10073 |
| C | 3.59847  | 3.26637  | -0.08657 |
| C | 5.73214  | -2.87602 | -0.12072 |
| C | 7.16422  | -2.85888 | -0.10954 |
| C | 7.84304  | -1.63271 | -0.09852 |
| C | 2.86861  | -2.88732 | -0.14651 |
| C | 3.57806  | -4.11963 | -0.14817 |
| C | 5.04345  | -4.12535 | -0.13332 |
| C | 5.78774  | -5.29818 | -0.13229 |
| C | 7.19474  | -5.27834 | -0.12069 |
| C | 7.87516  | -4.08766 | -0.11008 |
| C | 1.43727  | -0.42484 | -0.13885 |
| C | 0.72720  | -1.64351 | -0.15931 |
| C | 1.44046  | -2.88242 | -0.16329 |
| C | 0.73125  | -4.11124 | -0.18453 |
| C | 1.46095  | -5.30191 | -0.18245 |
| C | 2.84363  | -5.30503 | -0.16504 |
| C | 1.44467  | 2.03702  | -0.10491 |
| C | 0.73375  | 0.81768  | -0.12464 |
| C | -0.70745 | -1.63927 | -0.17353 |
| C | -1.42796 | -2.87369 | -0.19787 |
| C | -0.72671 | -4.10650 | -0.20648 |
| C | -1.40945 | -0.41658 | -0.14713 |
| C | -0.69855 | 0.82185  | -0.12515 |
| C | -2.84291 | -0.41297 | -0.14114 |
| C | -3.55643 | -1.62748 | -0.16473 |
| C | -2.85585 | -2.87008 | -0.19674 |
| C | -3.57306 | -4.09779 | -0.21887 |
| C | -2.84601 | -5.28763 | -0.23507 |
| C | -1.46327 | -5.29276 | -0.22753 |
| C | 2.91024  | 4.50572  | -0.07618 |
| C | 1.45245  | 4.50773  | -0.07149 |
| C | 0.73919  | 3.27847  | -0.08624 |
| C | -0.68927 | 3.28253  | -0.07995 |
| C | -1.40215 | 2.04520  | -0.09838 |
| C | -2.83577 | 2.04838  | -0.09122 |
| C | -3.54417 | 0.83087  | -0.11114 |
| C | -4.97672 | 0.83338  | -0.10355 |
| C | -5.68994 | -0.39447 | -0.12765 |
| C | -4.99465 | -1.62231 | -0.15947 |
| C | -5.71956 | -2.84126 | -0.18732 |
| C | -5.03850 | -4.09442 | -0.22099 |
| C | -7.12720 | -0.38007 | -0.12113 |
| C | -7.82284 | -1.58553 | -0.14921 |
| C | -7.15151 | -2.81539 | -0.18356 |
| C | -7.87003 | -4.03940 | -0.21566 |
| C | -7.19690 | -5.23371 | -0.25101 |
| C | -5.79001 | -5.26216 | -0.25404 |
| C | -7.80794 | 0.86467  | -0.08725 |
| C | -7.12328 | 2.05746  | -0.06332 |
| C | -5.68277 | 2.05353  | -0.07270 |
| C | -4.97334 | 3.28270  | -0.05130 |
| C | -3.54855 | 3.28702  | -0.06189 |
| C | -2.85290 | 4.52217  | -0.04263 |
| C | -1.39516 | 4.51584  | -0.05523 |
| C | -0.65822 | 5.70297  | -0.04276 |
| C | 0.72257  | 5.69904  | -0.05068 |
| C | -5.69113 | 4.50908  | -0.01966 |
| C | -7.13251 | 4.48959  | -0.00823 |
| C | -7.81545 | 3.32420  | -0.02911 |
| C | -4.97725 | 5.70813  | 0.00039  |
| C | -3.59299 | 5.71314  | -0.01093 |
| C | 5.04179  | 5.67953  | -0.06675 |
| C | 3.65754  | 5.69265  | -0.06856 |
| C | -0.74719 | -2.23084 | 3.11126  |
| C | -0.08159 | -0.87629 | 3.33490  |
| H | -0.68232 | -0.24409 | 3.99458  |
| H | -7.65621 | 5.44073  | 0.01793  |

|   |          |          |          |
|---|----------|----------|----------|
| H | 7.71920  | 5.39629  | -0.05831 |
| H | -8.90956 | -1.57448 | -0.14538 |
| H | -8.89478 | 0.86564  | -0.08105 |
| H | -8.90123 | 3.31271  | -0.02062 |
| H | -8.95531 | -4.00847 | -0.21283 |
| H | -7.74455 | -6.16977 | -0.27746 |
| H | -5.30436 | -6.22959 | -0.28515 |
| H | -3.35516 | -6.24307 | -0.24966 |
| H | -0.96370 | -6.25270 | -0.23735 |
| H | 0.95584  | -6.25889 | -0.19526 |
| H | 3.34702  | -6.26362 | -0.16596 |
| H | 5.29617  | -6.26307 | -0.14077 |
| H | 7.73671  | -6.21806 | -0.12061 |
| H | 8.96059  | -4.06338 | -0.10169 |
| H | 8.92980  | -1.62820 | -0.09096 |
| H | 8.92991  | 0.81279  | -0.07942 |
| H | 8.95128  | 3.26050  | -0.06607 |
| H | -5.52037 | 6.64816  | 0.02562  |
| H | -3.08910 | 6.67105  | 0.00702  |
| H | -1.15978 | 6.66192  | -0.02605 |
| H | 1.22979  | 6.65508  | -0.03792 |
| H | 3.15936  | 6.65370  | -0.06401 |
| H | 5.59061  | 6.61654  | -0.06011 |
| H | -0.89563 | -2.76003 | 4.05680  |
| H | -1.72530 | -2.11697 | 2.63246  |
| H | -0.13808 | -2.86833 | 2.46189  |
| H | 0.90587  | -0.99033 | 3.79082  |
| H | 0.04935  | -0.33932 | 2.39043  |

#### Ethane-convex surface of SWCNT, CPCM

|   |          |         |          |
|---|----------|---------|----------|
| C | -4.35400 | 3.13969 | 3.46679  |
| C | -4.37445 | 4.00253 | 2.30228  |
| C | -3.16420 | 4.25890 | 1.62780  |
| C | -1.91364 | 3.97755 | 2.26939  |
| C | -1.89330 | 3.14341 | 3.39856  |
| C | -3.12453 | 2.59104 | 3.88270  |
| C | -5.58230 | 4.34393 | 1.63005  |
| C | -5.59221 | 4.60369 | 0.28526  |
| C | -4.39468 | 4.53960 | -0.48277 |
| C | -3.17448 | 4.52831 | 0.22186  |
| C | -1.93327 | 4.50232 | -0.49478 |
| C | -1.93155 | 4.15374 | -1.85472 |
| C | -3.17142 | 3.82269 | -2.49390 |
| C | -4.39301 | 4.17420 | -1.88583 |
| C | -0.69679 | 4.56168 | 0.21404  |
| C | -0.68649 | 4.30163 | 1.61690  |
| C | -3.15777 | 2.89938 | -3.58721 |
| C | -4.36665 | 2.34417 | -4.05221 |
| C | -5.57619 | 2.96918 | -3.63517 |
| C | -5.58882 | 3.85354 | -2.58928 |
| C | -1.90490 | 2.34133 | -4.00552 |
| C | -0.67926 | 2.94601 | -3.59438 |
| C | -0.69304 | 3.86576 | -2.50271 |
| C | 0.52256  | 4.21059 | -1.87831 |
| C | 0.52060  | 4.56305 | -0.49548 |
| C | -4.34320 | 1.02212 | -4.64645 |
| C | -3.11265 | 0.34132 | -4.73620 |
| C | -1.88226 | 1.06094 | -4.58096 |
| C | -0.63397 | 0.38788 | -4.74345 |
| C | 0.57242  | 1.10419 | -4.60952 |
| C | 0.54944  | 2.40588 | -4.02414 |
| C | 1.77575  | 2.98835 | -3.58303 |
| C | 1.76228  | 3.89283 | -2.50972 |
| C | 1.75762  | 4.59979 | 0.21387  |
| C | 2.99787  | 4.62584 | -0.50464 |
| C | 3.00036  | 4.26442 | -1.88977 |
| C | 4.22055  | 4.01213 | -2.54796 |
| C | 4.23478  | 3.07819 | -3.65659 |
| C | 3.02803  | 2.45679 | -4.03483 |
| C | 3.05102  | 1.15205 | -4.62213 |
| C | 1.82098  | 0.42398 | -4.73601 |
| C | 4.28063  | 0.49279 | -4.81936 |
| C | 5.46458  | 1.28021 | -4.73641 |
| C | 5.44258  | 2.52875 | -4.17383 |
| C | 4.21588  | 4.73016 | 0.19635  |

C 5.41134 4.78875 -0.57532  
 C 5.41359 4.44199 -1.90020  
 C 4.22666 4.45790 1.62056  
 C 3.01887 4.09996 2.25182  
 C 1.76798 4.34036 1.59412  
 C 0.54094 4.04666 2.26116  
 C 4.30944 -0.95598 -4.77436  
 C 3.10616 -1.65021 -4.53820  
 C 1.84872 -0.97917 -4.69412  
 C 0.62755 -1.69875 -4.52601  
 C -0.60566 -1.03913 -4.70052  
 C -1.82675 -1.74945 -4.49708  
 C -3.08415 -1.08914 -4.69345  
 C -4.28704 -1.81114 -4.56228  
 C -5.50092 -1.10941 -4.81065  
 C -5.52816 0.25931 -4.85137  
 C 0.65431 -2.96335 -3.86374  
 C -0.55278 -3.52332 -3.39916  
 C -1.80035 -2.99331 -3.84599  
 C -3.03089 -3.57319 -3.39292  
 C -4.25969 -3.09519 -3.89015  
 C 0.56148 3.19860 3.40974  
 C -0.64568 2.63780 3.87348  
 C 1.90150 -3.47005 -3.38966  
 C 3.13270 -2.91825 -3.87482  
 C 3.03972 3.24872 3.40238  
 C 1.80925 2.66872 3.85599  
 C 4.36218 -3.46800 -3.46077  
 C 5.54880 -2.90235 -4.00836  
 C 5.52353 -1.68862 -4.64248  
 C 4.26865 2.77040 3.89892  
 C 5.45338 3.41528 3.44240  
 C 5.43297 4.23066 2.34213  
 C -0.61867 1.37267 4.53452  
 C 0.61484 0.71319 4.70802  
 C 1.83582 1.42403 4.50559  
 C 3.09337 0.76354 4.70066  
 C 4.29617 1.48581 4.57015  
 C -3.09753 1.32289 4.54581  
 C -1.83969 0.65240 4.70147  
 C -1.81139 -0.75078 4.74134  
 C -0.56267 -1.43040 4.61362  
 C 0.64343 -1.71391 4.74846  
 C 1.89177 -1.38650 4.58492  
 C 3.12203 -0.66697 4.74130  
 C 4.35264 -1.34755 4.65085  
 C 5.53751 -0.58486 4.85663  
 C 5.51014 0.78391 4.81751  
 C -0.53946 -2.73164 4.02713  
 C 0.68912 -3.27114 3.59654  
 C 1.91451 -2.66623 4.00807  
 C 3.16739 -3.22420 3.59024  
 C 4.37617 -2.66923 4.05587  
 C -5.54074 2.57313 4.01325  
 C -5.51504 1.35960 4.64774  
 C -4.30051 0.62782 4.78085  
 C -4.27091 -0.82093 4.82568  
 C -3.04102 -1.47943 4.62737  
 C -3.01761 -2.78412 4.03995  
 C -1.76539 -3.31519 3.58711  
 C -1.75189 -4.22162 2.51520  
 C -0.51252 -4.54190 1.88425  
 C 0.70277 -4.19275 2.50646  
 C 1.94146 -4.48186 1.85933  
 C 3.18110 -4.14837 2.49774  
 C 4.40300 -4.50025 1.89058  
 C 5.59865 -4.17934 2.59418  
 C 5.58581 -3.29452 3.63963  
 C -0.51090 -4.90267 0.50284  
 C 0.70604 -4.90243 -0.20764  
 C 1.94314 -4.83697 0.50098  
 C 3.18434 -4.85842 -0.21607  
 C 4.40484 -4.86656 0.48801  
 C -5.45440 -1.60910 4.74401  
 C -5.43199 -2.85784 4.18193

C -4.22433 -3.40654 3.66361  
 C -4.21053 -4.34095 2.55545  
 C -2.99072 -4.59386 1.89684  
 C -2.98907 -4.95508 0.51179  
 C -1.74872 -4.93250 -0.20682  
 C -1.75934 -4.66748 -1.58568  
 C -0.53204 -4.37319 -2.25204  
 C 0.69513 -4.63310 -1.60978  
 C 1.92184 -4.30640 -2.26181  
 C 3.17322 -4.58848 -1.62174  
 C 4.38307 -4.33128 -2.29665  
 C 5.59158 -4.67143 -1.62506  
 C 5.60230 -4.92971 -0.28009  
 C -5.40421 -4.76988 1.90821  
 C -5.40281 -5.11522 0.58305  
 C -4.20747 -5.05692 -0.18881  
 C -4.21820 -4.78348 -1.61253  
 C -3.01011 -4.42504 -2.24291  
 C -5.42438 -4.55596 -2.33426  
 C -5.44456 -3.74024 -3.43423  
 C 0.30894 -7.94984 0.38890  
 C -0.75724 7.84014 -0.69785  
 H 1.30587 8.07080 -0.04474  
 H 6.49694 -1.08244 4.94061  
 H 6.44883 1.32367 4.87019  
 H 6.40879 3.18289 3.89888  
 H 6.37294 4.61604 1.96394  
 H 6.35819 5.00544 -0.09386  
 H 6.36202 4.39611 -2.42324  
 H 6.38210 3.05057 -4.03204  
 H 6.42041 0.85573 -5.02189  
 H 6.46330 -1.24262 -4.94782  
 H 6.50773 -3.37680 -3.83364  
 H 6.53746 -4.62355 -2.15252  
 H 6.55674 -5.07843 0.21183  
 H 6.55336 -4.55093 2.23985  
 H 6.53106 -2.99523 4.07803  
 H -6.52850 4.29675 2.15705  
 H -6.54634 4.75435 -0.20667  
 H -6.54353 4.22460 -2.23440  
 H -6.52160 2.66978 -4.07314  
 H -6.48751 0.75691 -4.93599  
 H -6.43966 -1.64914 -4.86283  
 H -6.39980 -3.50793 -3.89111  
 H -6.36436 -4.94174 -1.95649  
 H -6.34998 -5.33051 0.10160  
 H -6.35233 -4.72368 2.43176  
 H -6.37122 -3.38057 4.04154  
 H -6.41021 -1.18530 5.03056  
 H -6.45477 0.91281 4.95201  
 H -6.49993 3.04659 3.83717  
 H 0.12117 8.80862 1.03935  
 H 0.32956 7.05528 1.01917  
 H -1.74511 7.65273 -0.26604  
 H -0.81724 8.76087 -1.28492  
 H -0.54013 7.01901 -1.38820

# Methane-concave surface of SWCNT, CPCM

C 4.31135 1.75878 4.47833  
 C 4.30843 0.34238 4.78721  
 C 3.08949 -0.36203 4.72682  
 C 1.84785 0.35414 4.70812  
 C 1.85082 1.72603 4.40959  
 C 3.09558 2.37897 4.12805  
 C 5.50578 -0.42625 4.84438  
 C 5.50255 -1.76114 4.53816  
 C 4.30213 -2.42202 4.15147  
 C 3.08629 -1.75687 4.40582  
 C 1.84186 -2.38792 4.07632  
 C 1.83949 -3.48984 3.20640  
 C 3.08230 -3.95766 2.66662  
 C 4.29999 -3.55920 3.25278  
 C 0.60799 -1.74852 4.40005  
 C 0.61104 -0.35744 4.72033

C -0.61247 -2.38357 4.09593  
 C -0.61476 -3.50581 3.21312  
 C 0.60330 -3.95256 2.66310  
 C 0.60157 -4.58234 1.38192  
 C 1.83714 -4.72366 0.68109  
 C 3.08126 -4.58514 1.38071  
 C 4.29822 -4.79851 0.70359  
 C 5.49739 -4.68933 1.46415  
 C 5.49814 -4.09047 2.69588  
 C 1.83716 -4.71723 -0.72298  
 C 3.08132 -4.57237 -1.42128  
 C 4.29823 -4.79201 -0.74611  
 C 0.60164 -4.56949 -1.42255  
 C -0.61771 -4.73250 -0.73519  
 C -0.61774 -4.73903 0.69302  
 C -1.85270 -4.55385 1.38463  
 C -1.85139 -3.93763 2.64617  
 C -3.09356 -3.50262 3.21539  
 C -3.09102 -2.37970 4.10244  
 C -1.84629 -1.72897 4.38887  
 C -1.84354 -0.36062 4.70324  
 C -0.60689 0.35099 4.72483  
 C -0.60389 1.74598 4.42163  
 C 0.61691 2.38357 4.12340  
 C 0.60343 -3.92806 -2.69794  
 C 1.83966 -3.46049 -3.23698  
 C 3.08244 -3.93318 -2.70139  
 C 4.30017 -3.52952 -3.28390  
 C 5.49825 -4.06601 -2.73185  
 C 5.49741 -4.67612 -1.50567  
 C -3.09728 -4.72837 0.69441  
 C -3.09724 -4.72185 -0.73661  
 C -1.85263 -4.54099 -1.42514  
 C -1.85126 -3.91327 -2.68097  
 C -0.61460 -3.47638 -3.24394  
 C -0.61226 -2.34635 -4.11672  
 C 0.60822 -1.70866 -4.41519  
 C 1.84208 -2.35090 -4.09706  
 C 3.08653 -1.71700 -4.42096  
 C 4.30236 -2.38438 -4.17245  
 C -4.31421 -4.61998 1.39640  
 C -4.31238 -3.98705 2.70034  
 C -1.84606 -1.68919 -4.40395  
 C -3.09081 -2.34242 -4.12335  
 C -3.09340 -3.47315 -3.24631  
 C -4.31225 -3.96222 -2.73575  
 C -4.31415 -4.60704 -1.43765  
 C -5.51383 -4.83959 -0.70648  
 C -5.51386 -4.84581 0.66308  
 C -4.30674 -1.76358 4.45996  
 C -5.50704 -2.47948 4.18735  
 C -5.50996 -3.55294 3.33674  
 C -4.30415 -0.35039 4.78323  
 C -3.08541 0.35495 4.73073  
 C -3.08242 1.75332 4.42541  
 C -1.83792 2.38835 4.10393  
 C -4.30651 -1.72318 -4.47552  
 C -5.50683 -2.44146 -4.20933  
 C -5.50980 -3.52245 -3.36831  
 C -4.29832 2.42032 4.17600  
 C -5.49876 1.75516 4.55527  
 C -5.50172 0.41728 4.84812  
 C 0.61934 3.51093 3.24769  
 C -0.59920 3.96143 2.70146  
 C -1.83563 3.49672 3.24222  
 C -3.07808 3.96815 2.70428  
 C -4.29601 3.56500 3.28671  
 C 3.09805 3.50881 3.24967  
 C 1.85577 3.94741 2.68398  
 C 1.85716 4.57108 1.42608  
 C 0.62202 4.75661 0.73512  
 C -0.59778 4.59588 1.42251  
 C -1.83298 4.74549 0.72303  
 C -3.07682 4.60389 1.42208  
 C -4.29363 4.82286 0.74625

C -5.49289 4.70830 1.50593  
 C -5.49399 4.10023 2.73315  
 C 0.62206 4.76313 -0.69278  
 C -0.59770 4.60874 -1.38169  
 C -1.83294 4.75192 -0.68094  
 C -3.07676 4.61670 -1.38131  
 C -4.29361 4.82938 -0.70354  
 C 5.51182 2.47643 4.21078  
 C 5.51456 3.55692 3.36912  
 C 4.31667 3.99669 2.73708  
 C 4.31815 4.64001 1.43812  
 C 3.10115 4.75344 0.73694  
 C 3.10119 4.75995 -0.69447  
 C 1.85725 4.58393 -1.38533  
 C 1.85593 3.97181 -2.64890  
 C 0.61953 3.54042 -3.21660  
 C -0.59904 3.98602 -2.66641  
 C -1.83543 3.52620 -3.21141  
 C -3.07792 3.99274 -2.66929  
 C -4.29581 3.59478 -3.25539  
 C -5.49386 4.12479 -2.69699  
 C -5.49285 4.72157 -1.46423  
 C 0.61715 2.42084 -4.10225  
 C -0.60364 1.78591 -4.40615  
 C -1.83768 2.42548 -4.08291  
 C -3.08216 1.79329 -4.41000  
 C -4.29806 2.45807 -4.15479  
 C 5.51763 4.87305 0.70665  
 C 5.51767 4.87927 -0.66293  
 C 4.31824 4.65293 -1.39657  
 C 4.31683 4.02148 -2.70135  
 C 3.09824 3.53827 -3.21842  
 C 3.09582 2.41624 -4.10677  
 C 1.85107 1.76583 -4.39413  
 C 1.84811 0.39661 -4.70473  
 C 0.61129 -0.31482 -4.72325  
 C -0.60663 0.39363 -4.72160  
 C -1.84329 -0.31814 -4.70629  
 C -3.08515 0.39764 -4.72758  
 C -4.30390 -0.30719 -4.78629  
 C -5.50147 0.46101 -4.84443  
 C -5.49850 1.79628 -4.53985  
 C 5.51476 3.58734 -3.33721  
 C 5.51205 2.51439 -4.18844  
 C 4.31160 1.79915 -4.46243  
 C 4.30868 0.38553 -4.78383  
 C 3.08974 -0.31938 -4.72967  
 C 5.50602 -0.38259 -4.84780  
 C 5.50279 -1.72011 -4.55334  
 C -0.19006 -1.47489 -0.00596  
 H -0.01528 -0.39828 -0.00104  
 H -6.44114 5.00547 1.07256  
 H -6.44329 3.93609 3.23015  
 H -6.44664 2.27939 4.51153  
 H -6.45221 -0.07257 5.02630  
 H -6.45458 -2.11566 4.56800  
 H -6.45986 -4.00333 3.07204  
 H -6.46309 -4.91737 1.18178  
 H -6.46303 -4.90644 -1.22585  
 H -6.45972 -3.97519 -3.10770  
 H -6.45434 -2.07426 -4.58680  
 H -6.45196 -0.02724 -5.02691  
 H -6.44636 2.32013 -4.49143  
 H -6.44313 3.96493 -3.19544  
 H -6.44115 5.01455 -1.02814  
 H 6.45631 0.06150 5.02803  
 H 6.45022 -2.28533 4.48995  
 H 6.44726 -3.92992 3.19439  
 H 6.44573 -4.98295 1.02858  
 H 6.44570 -4.97391 -1.07281  
 H 6.44739 -3.90119 -3.22890  
 H 6.45047 -2.24468 -4.50984  
 H 6.45655 0.10677 -5.02714  
 H 6.45979 2.15009 -4.56815  
 H 6.46470 4.03690 -3.07126

H 6.46690 4.95182 -1.18150  
 H 6.46682 4.94092 1.22592  
 H 6.46452 4.00884 3.10725  
 H 6.45953 2.10877 4.58730  
 H 0.76651 -2.00347 -0.00852  
 H -0.75669 -1.75914 0.88443  
 H -0.75692 -1.75095 -0.89880

#### Methane-graphene, CPCM

C 3.65249 5.67271 -0.00611  
 C 2.90621 4.48520 -0.02047  
 C 3.59542 3.24639 -0.02916  
 C 5.02019 3.23488 -0.02210  
 C 5.74435 4.45782 -0.00685  
 C 5.03672 5.66071 0.00051  
 C 5.72322 2.00191 -0.03020  
 C 7.16373 1.99849 -0.02239  
 C 7.86251 3.26196 -0.00633  
 C 7.18562 4.43106 0.00094  
 C 2.87614 2.01119 -0.04478  
 C 3.57824 0.78990 -0.05337  
 C 5.01084 0.78514 -0.04562  
 C 5.71771 -0.44652 -0.05381  
 C 7.15503 -0.43958 -0.04539  
 C 7.84222 0.80196 -0.02988  
 C 2.87052 -0.45047 -0.06971  
 C 3.57778 -1.66866 -0.07755  
 C 5.01598 -1.67100 -0.06946  
 C 5.73446 -2.89399 -0.07587  
 C 7.16654 -2.87566 -0.06609  
 C 7.84433 -1.64896 -0.05184  
 C 5.04677 -4.14387 -0.09045  
 C 3.58135 -4.13929 -0.10308  
 C 2.87082 -2.90763 -0.09354  
 C 1.44260 -2.90383 -0.10177  
 C 0.72828 -1.66568 -0.10060  
 C 1.43709 -0.44665 -0.08055  
 C 0.73253 0.79523 -0.06938  
 C 1.44256 2.01522 -0.05229  
 C 0.73619 3.25626 -0.04138  
 C 1.44844 4.48611 -0.02612  
 C 5.79201 -5.31610 -0.09083  
 C 7.19901 -5.29508 -0.08144  
 C 7.87848 -4.10387 -0.07024  
 C 0.73460 -4.13324 -0.11314  
 C 1.46517 -5.32319 -0.13199  
 C 2.84797 -5.32519 -0.12765  
 C -0.69960 0.79828 -0.07769  
 C -1.40933 -0.44032 -0.09719  
 C -0.70630 -1.66246 -0.11460  
 C -1.42569 -2.89745 -0.11258  
 C -0.72335 -4.12994 -0.10727  
 C -0.69229 3.25940 -0.04569  
 C -1.40412 2.02148 -0.06147  
 C -2.84260 -0.43768 -0.08897  
 C -3.55533 -1.65297 -0.09226  
 C -2.85373 -2.89515 -0.10407  
 C -3.56984 -4.12373 -0.09959  
 C -2.84173 -5.31294 -0.08612  
 C -1.45891 -5.31682 -0.08776  
 C -3.54509 0.80571 -0.07206  
 C -2.83769 2.02388 -0.06150  
 C -4.97769 0.80719 -0.06684  
 C -5.68996 -0.42144 -0.07416  
 C -4.99361 -1.64899 -0.08567  
 C -5.71747 -2.86883 -0.09308  
 C -5.03528 -4.12175 -0.10430  
 C -1.39910 4.49241 -0.03380  
 C -0.66310 5.68007 -0.01960  
 C 0.71769 5.67702 -0.01601  
 C -2.85687 4.49796 -0.03560  
 C -3.55153 3.26222 -0.04732  
 C -4.97634 3.25696 -0.04498  
 C -5.68476 2.02704 -0.05398  
 C -7.12529 2.02995 -0.04969

C -7.80901 0.83640 -0.05786  
 C -7.12725 -0.40816 -0.07021  
 C -7.82186 -1.61451 -0.07965  
 C -7.14946 -2.84417 -0.09204  
 C -7.86682 -4.06920 -0.10507  
 C -7.19259 -5.26332 -0.12096  
 C -5.78566 -5.29058 -0.12152  
 C -5.69511 4.48306 -0.03239  
 C -7.13652 4.46262 -0.02878  
 C -7.81852 3.29651 -0.03681  
 C -4.98221 5.68284 -0.02326  
 C -3.59792 5.68875 -0.02468  
 C -0.73233 -1.68599 3.15098  
 H -1.75636 -1.68278 2.77234  
 H -7.66107 5.41359 -0.01881  
 H 7.71429 5.37972 0.01324  
 H -8.90860 -1.60430 -0.07805  
 H -8.89586 0.83663 -0.05484  
 H -8.90432 3.28433 -0.03359  
 H -8.95214 -4.03927 -0.10418  
 H -7.73946 -6.20011 -0.13404  
 H -5.29904 -6.25787 -0.13888  
 H -3.35007 -6.26877 -0.06860  
 H -0.95848 -6.27618 -0.06885  
 H 0.96074 -6.28036 -0.15474  
 H 3.35219 -6.28319 -0.14537  
 H 5.30120 -6.28138 -0.09749  
 H 7.74176 -6.23436 -0.08295  
 H 8.96390 -4.07873 -0.06321  
 H 8.93108 -1.64354 -0.04495  
 H 8.92905 0.79744 -0.02369  
 H 8.94823 3.24501 -0.00018  
 H -5.52618 6.62267 -0.01420  
 H -3.09476 6.64717 -0.01653  
 H -1.16543 6.63872 -0.01018  
 H 1.22420 6.63344 -0.00403  
 H 3.15352 6.63334 0.00038  
 H 5.58476 6.59815 0.01194  
 H -0.74355 -1.69563 4.24140  
 H -0.21475 -2.57314 2.78082  
 H -0.21452 -0.79275 2.79612

#### Methane-convex surface of SWCNT, CPCM

C -3.97629 -2.00346 4.69354  
 C -4.20412 -0.58220 4.86589  
 C -3.11468 0.30033 4.72707  
 C -1.77315 -0.20394 4.77075  
 C -1.55242 -1.58054 4.60429  
 C -2.67337 -2.44960 4.39446  
 C -5.51023 -0.01489 4.85683  
 C -5.72022 1.26286 4.41059  
 C -4.63866 2.06278 3.94335  
 C -3.33398 1.63584 4.26155  
 C -2.20427 2.41992 3.85625  
 C -2.37081 3.39978 2.86424  
 C -3.66632 3.59177 2.28083  
 C -4.81051 3.07450 2.91952  
 C -0.88631 2.02858 4.23922  
 C -0.66751 0.69623 4.70341  
 C 0.21883 2.81463 3.85506  
 C 0.04923 3.81180 2.84703  
 C -1.21938 3.98587 2.25839  
 C -1.30580 4.44499 0.90921  
 C -2.53897 4.29868 0.20720  
 C -3.75238 4.05166 0.92831  
 C -4.98077 3.99127 0.24118  
 C -6.15454 3.78061 1.01945  
 C -6.07209 3.33657 2.31268  
 C -2.52410 4.13934 -1.18693  
 C -3.72297 3.73168 -1.85815  
 C -4.96569 3.82598 -1.19978  
 C -1.27587 4.12345 -1.87750  
 C -0.10543 4.55506 -1.22161  
 C -0.12096 4.71860 0.19718



C -2.02571 4.52728 -1.49012  
 C -0.79255 4.75708 -0.80922  
 C -0.78576 4.78889 0.61831  
 C 0.44103 4.67696 1.30287  
 C 1.66880 4.84032 0.59327  
 C 2.91919 4.74853 1.28883  
 C 4.12691 4.98191 0.60157  
 C 0.46448 4.07518 2.59707  
 C 1.71491 3.65505 3.14160  
 C 2.94247 4.14444 2.58591  
 C 4.17291 3.78723 3.17154  
 C 5.35407 4.34030 2.59953  
 C 5.33210 4.91803 1.35815  
 C -3.27071 4.68917 -0.79776  
 C -3.26381 4.72140 0.63325  
 C -2.01229 4.58907 1.32031  
 C -1.98919 3.99800 2.59356  
 C -0.73942 3.60779 3.16134  
 C -0.70421 2.50450 4.06649  
 C 0.53354 1.90471 4.37266  
 C 1.74934 2.56900 4.03015  
 C 3.01110 1.97413 4.36055  
 C 4.20862 2.66528 4.08819  
 C 0.57353 0.51931 4.71407  
 C 1.82699 -0.16216 4.70331  
 C 3.05077 0.58477 4.70181  
 C 4.28744 -0.08757 4.76509  
 C 5.46565 0.71140 4.80341  
 C 5.42749 2.04089 4.47756  
 C -3.21725 3.54325 3.17752  
 C -3.18184 2.43894 4.08723  
 C -1.91957 1.82480 4.37886  
 C -1.88012 0.46237 4.71633  
 C -0.62627 -0.21897 4.73990  
 C -0.58983 -1.61835 4.46043  
 C 0.64294 -2.23292 4.16699  
 C 1.86133 -1.53862 4.42917  
 C 3.12051 -2.16453 4.15186  
 C 4.32321 -1.50836 4.48120  
 C 5.56289 -3.29869 3.40120  
 C 5.53949 -2.20152 4.22010  
 C -3.10420 -0.28252 4.76455  
 C -3.06796 -1.68498 4.48110  
 C -1.81020 -2.29413 4.16122  
 C -4.26898 -2.38456 4.24934  
 C -5.48293 -1.74437 4.62807  
 C -5.51754 -0.40255 4.90014  
 C -4.33981 0.39320 4.81315  
 C -4.38010 1.79940 4.46275  
 C -5.59939 2.47900 4.18139  
 C -5.63340 3.53502 3.30967  
 C -4.45018 3.98701 2.65923  
 C -4.47415 4.59540 1.34364  
 C -5.68251 4.77804 0.61250  
 C -5.68914 4.74714 -0.75679  
 C -4.48767 4.53215 -1.49040  
 C -4.47575 3.86661 -2.77830  
 C -5.66456 3.38585 -3.39732  
 C -5.63821 2.29290 -4.22250  
 C -4.42125 1.60181 -4.48495  
 O 0.35036 -1.34723 1.15739  
 C 0.51637 -1.15606 -0.04114  
 N -0.50319 -1.21700 -0.93263  
 C 1.87152 -0.80516 -0.63822  
 C 2.99325 -0.91122 0.38516  
 H 6.26084 5.17870 -1.18788  
 H 6.27947 4.07353 -3.32684  
 H 6.31799 2.39824 -4.58030  
 H 6.38322 0.03739 -5.05177  
 H 6.44292 -1.99213 -4.54590  
 H 6.49887 -3.85016 -3.01499  
 H 6.52683 -4.74815 -1.12352  
 H 6.53521 -4.70265 1.28443  
 H 6.52168 -3.73324 3.14208  
 H 6.48037 -1.80409 4.58340

H 6.42893 0.24974 4.98846  
 H 6.36161 2.58750 4.41654  
 H 6.30947 4.21426 3.09596  
 H 6.27021 5.23041 0.91343  
 H -6.52370 -0.15613 -5.00834  
 H -6.45717 -2.49408 -4.43732  
 H -6.41010 -4.10985 -3.10111  
 H -6.37394 -5.11127 -0.91173  
 H -6.36616 -5.05568 1.18792  
 H -6.38303 -3.95787 3.33063  
 H -6.41739 -2.29319 4.60004  
 H -6.47849 0.06671 5.07777  
 H -6.53606 2.09876 4.57288  
 H -6.59575 3.95507 3.04002  
 H -6.63066 4.83548 1.13498  
 H -6.64220 4.78093 -1.27235  
 H -6.62455 3.81770 -3.13809  
 H -6.57815 1.89664 -4.58936  
 H 3.95438 -0.66170 -0.07074  
 H 2.81710 -0.23580 1.22724  
 H 3.05112 -1.92667 0.78641  
 H 1.80403 0.21082 -1.04838  
 H 2.05575 -1.46516 -1.49513  
 H -0.36200 -1.06232 -1.91961  
 H -1.42786 -1.45346 -0.60496

#### Propanamide-graphene, CPCM

C 3.70246 5.62534 -0.17113  
 C 2.96052 4.43522 -0.19045  
 C 3.65422 3.19878 -0.18752  
 C 5.07890 3.19214 -0.16506  
 C 5.79852 4.41769 -0.14572  
 C 5.08659 5.61806 -0.14888  
 C 5.78631 1.96161 -0.16384  
 C 7.22670 1.96309 -0.14376  
 C 7.92076 3.22912 -0.12347  
 C 7.23975 4.39586 -0.12409  
 C 2.93945 1.96104 -0.20623  
 C 3.64598 0.74219 -0.20361  
 C 5.07836 0.74232 -0.18133  
 C 5.78942 -0.48706 -0.18018  
 C 7.22669 -0.47516 -0.16304  
 C 7.90936 0.76889 -0.14470  
 C 2.94279 -0.50069 -0.21634  
 C 3.65385 -1.71668 -0.21057  
 C 5.09193 -1.71407 -0.19391  
 C 5.81458 -2.93472 -0.19272  
 C 7.24657 -2.91133 -0.18031  
 C 7.92006 -1.68225 -0.16488  
 C 5.13121 -4.18706 -0.20419  
 C 3.66569 -4.18750 -0.20968  
 C 2.95106 -2.95824 -0.21408  
 C 1.52292 -2.95971 -0.22018  
 C 0.80448 -1.72390 -0.23804  
 C 1.50951 -0.50158 -0.24181  
 C 0.79989 0.73785 -0.25154  
 C 1.50598 1.96027 -0.23579  
 C 0.79535 3.19903 -0.24417  
 C 1.50295 4.43107 -0.21736  
 C 5.88045 -5.35672 -0.20770  
 C 7.28736 -5.33069 -0.19783  
 C 7.96269 -4.13716 -0.18343  
 C 0.81872 -4.19112 -0.20860  
 C 1.55321 -5.37880 -0.20945  
 C 2.93606 -5.37599 -0.21050  
 C -0.63202 0.73625 -0.28306  
 C -1.33749 -0.50439 -0.27073  
 C -0.63041 -1.72501 -0.25404  
 C -1.34565 -2.96248 -0.23057  
 C -0.63914 -4.19218 -0.19928  
 C -0.63337 3.19672 -0.28054  
 C -1.34107 1.95665 -0.29617  
 C -2.77069 -0.50603 -0.28105  
 C -3.47890 -1.72378 -0.26248

C -2.77373 -2.96420 -0.23599  
 C -3.48586 -4.19466 -0.20833  
 C -2.75407 -5.38087 -0.16088  
 C -1.37124 -5.38056 -0.15597  
 C -3.47649 0.73421 -0.30143  
 C -2.77345 1.95419 -0.31098  
 C -4.90844 0.73082 -0.31400  
 C -5.61723 -0.49985 -0.30010  
 C -4.91724 -1.72492 -0.27272  
 C -5.63715 -2.94702 -0.25713  
 C -4.95120 -4.19752 -0.22762  
 C -1.34413 4.42786 -0.28432  
 C -0.61241 5.61813 -0.24687  
 C 0.76782 5.61965 -0.21574  
 C -2.80119 4.42819 -0.32233  
 C -3.49103 3.18969 -0.32602  
 C -4.91577 3.18017 -0.34597  
 C -5.62004 1.94812 -0.33850  
 C -7.06045 1.94628 -0.35506  
 C -7.74042 0.75060 -0.34330  
 C -7.05446 -0.49139 -0.31463  
 C -7.74528 -1.69985 -0.30127  
 C -7.06909 -2.92722 -0.27315  
 C -7.78268 -4.15442 -0.26140  
 C -7.10482 -5.34636 -0.23759  
 C -5.69789 -5.36882 -0.22171  
 C -5.63850 4.40383 -0.37091  
 C -7.07968 4.37864 -0.39113  
 C -7.75785 3.21026 -0.38328  
 C -4.92971 5.60613 -0.37652  
 C -3.54570 5.61656 -0.35220  
 C -0.40408 -0.45968 3.06522  
 C -1.09040 0.88068 2.85756  
 C -1.39454 -1.60998 3.16052  
 H -7.60717 5.32780 -0.41246  
 H 7.76503 5.34636 -0.10840  
 H -8.83200 -1.69321 -0.31303  
 H -8.82722 0.74711 -0.35513  
 H -8.84352 3.19433 -0.39759  
 H -8.86803 -4.12793 -0.27326  
 H -7.64868 -6.28496 -0.23124  
 H -5.20819 -6.33458 -0.20649  
 H -3.25949 -6.33772 -0.12399  
 H -0.86810 -6.33778 -0.11339  
 H 1.05184 -6.33784 -0.21320  
 H 3.44350 -6.33247 -0.21023  
 H 5.39300 -6.32367 -0.21886  
 H 7.83344 -6.26804 -0.20119  
 H 9.04801 -4.10833 -0.17468  
 H 9.00676 -1.67315 -0.15392  
 H 8.99613 0.76816 -0.13087  
 H 9.00645 3.21605 -0.10762  
 H -5.47655 6.54405 -0.39967  
 H -3.04541 6.57653 -0.35941  
 H -1.11835 6.57489 -0.23840  
 H 1.27066 6.57766 -0.18688  
 H 3.20020 6.58426 -0.17515  
 H 5.63125 6.55743 -0.13446  
 H -1.99971 -1.52972 4.06681  
 H -2.07503 -1.60002 2.30570  
 H -0.86998 -2.56846 3.17789  
 H 0.21662 -0.39462 3.96593  
 H 0.29135 -0.60933 2.22978  
 N -0.25973 1.95568 2.85891  
 O -2.30193 0.99217 2.71708  
 H 0.74170 1.84099 2.82933  
 H -0.63976 2.84972 2.58360

#### Propanamide-convex surface of SWCNT, CPCM

C 0.04314 -5.51636 -4.83914  
 C 0.87750 -4.39612 -4.56224  
 C 0.30562 -3.11484 -4.69504  
 C -1.11631 -2.97330 -4.77045  
 C -1.93989 -4.11544 -4.71163



C -1.31783 -5.38088 -4.91115  
 C 1.10533 -1.94609 -4.47091  
 C 2.33026 -2.07222 -3.79648  
 C 2.75173 -3.36690 -3.34638  
 C 2.14200 -4.52620 -3.86528  
 C 3.57765 -3.45668 -2.18107  
 C 3.78035 -4.70362 -1.55679  
 C 3.42475 -5.86847 -2.29483  
 C 2.63311 -5.78267 -3.40908  
 C 3.95071 -2.24834 -1.50567  
 C 3.81811 -0.98894 -2.16508  
 C 2.99570 -0.89971 -3.32843  
 C 2.59107 0.36952 -3.78854  
 C 1.34491 0.49758 -4.47335  
 C 0.54856 -0.64755 -4.67463  
 C -0.87000 -0.50667 -4.74932  
 C -1.68952 -0.66786 -4.61857  
 C 4.18492 -2.28083 -0.12184  
 C 4.05344 -3.52178 0.58359  
 C 4.02806 -4.73747 -0.12825  
 C 4.20760 0.19332 -1.50418  
 C 4.44082 0.16002 -0.09648  
 C 4.28738 -1.05395 0.60032  
 C 3.91057 -1.02498 1.97711  
 C 3.43385 -2.22347 2.58764  
 C 3.67002 -3.49208 1.96246  
 C 3.26190 -4.67934 2.60232  
 C 3.56377 -5.90920 1.95101  
 C 3.93465 -5.93748 0.63291  
 C 4.04381 1.45564 -2.14941  
 C 3.23277 1.54398 -3.29204  
 C 3.69394 0.21764 2.60523  
 C 4.13898 1.41877 1.97582  
 C 4.51363 1.38894 0.62406  
 C 4.70168 2.62322 -0.07897  
 C 4.46117 2.65819 -1.49032  
 C 4.36313 3.89605 -2.15582  
 C 3.52202 3.98844 -3.33292  
 C 2.83870 2.83637 -3.77112  
 C 1.58932 2.96482 -4.45773  
 C 0.77831 1.79682 -4.64183  
 C -0.61681 1.93529 -4.71533  
 C -1.44236 0.77484 -4.62025  
 C 3.94100 2.68409 2.61968  
 C 4.44837 3.86015 2.03196  
 C 4.84598 3.82739 0.63818  
 C 5.07495 5.01369 -0.11668  
 C 4.84012 5.04745 -1.46573  
 C 1.04690 4.24379 -4.69444  
 C 1.91399 5.36174 -4.53335  
 C 3.10893 5.23868 -3.87508  
 C -0.39331 4.38634 -4.77270  
 C -1.19757 3.24158 -4.60648  
 C -2.75345 0.90092 -4.06889  
 C -3.20001 2.18364 -3.63036  
 C -2.51217 3.36786 -4.05423  
 C -2.99729 4.63654 -3.67969  
 C -2.29556 5.77492 -4.16889  
 C -1.03753 5.65417 -4.69636  
 C -2.97896 -1.54377 -4.07608  
 C -3.44592 -0.25870 -3.66659  
 C -4.38969 -0.17219 -2.59875  
 C -4.60739 1.07049 -1.97062  
 C -4.12784 2.26869 -2.57993  
 C -4.36506 3.53748 -1.95598  
 C -3.95488 4.72447 -2.59509  
 C -4.99549 1.10009 -0.59693  
 C -4.89284 2.32637 0.12604  
 C -4.75406 3.56711 -0.57874  
 C -4.72579 4.78258 0.13338  
 C -4.62826 5.98298 -0.62669  
 C -4.25598 5.95476 -1.94419  
 C -3.69195 -2.72516 -3.68685  
 C -4.63817 -2.63847 -2.61643  
 C -4.83819 -1.37347 -1.97209

C -5.21999 -1.34424 -0.62113  
 C -5.15288 -0.11455 0.10003  
 C -4.90935 -0.14920 1.50654  
 C -4.51757 1.03272 2.16640  
 C -4.65410 2.29241 1.50932  
 C -4.27778 3.49984 2.18451  
 C -4.48029 4.74768 1.56171  
 C -3.69104 0.94301 3.32698  
 C -3.02630 2.11547 3.79634  
 C -3.44965 3.40998 3.34842  
 C -2.84052 4.56933 3.86816  
 C -3.33364 5.82601 3.41462  
 C -4.12575 1.50120 2.30093  
 C -5.40187 -2.58056 0.08166  
 C -5.15714 -2.61552 1.49152  
 C -4.73971 -1.41203 2.14955  
 C -3.92623 -1.50047 3.29053  
 C -3.28502 -0.32594 3.78663  
 C -2.03926 -0.45344 4.47255  
 C -1.24379 0.69194 4.67513  
 C -1.80134 1.99003 4.47104  
 C -1.00261 3.15915 4.69629  
 C -1.57543 4.44002 4.56385  
 C 0.17465 0.55172 4.75283  
 C 0.99371 1.71340 4.62253  
 C 0.41943 3.01859 4.77261  
 C 1.24225 4.16131 4.71335  
 C 0.61927 5.42641 4.91241  
 C -0.74176 5.56090 4.84066  
 C -3.53140 -2.79255 3.77034  
 C -2.28275 -2.92045 4.45828  
 C -1.47235 -1.75223 4.64279  
 C -0.07735 -1.89034 4.71986  
 C 0.74794 -0.72967 4.62614  
 C 2.06011 -0.85569 4.07719  
 C 2.75205 0.30420 3.67448  
 C 2.28385 1.58964 4.08188  
 C 2.99571 2.77129 3.69084  
 C 2.57297 4.03364 4.15268  
 C 4.25076 5.08097 2.73775  
 C 3.34531 5.16470 3.76215  
 C 0.50394 -3.19664 4.61271  
 C 1.81927 -3.32298 4.06228  
 C 2.50730 -2.13851 3.63920  
 C 2.30475 -4.59160 3.68768  
 C 1.60259 -5.73000 4.17600  
 C 0.34396 -5.60923 4.70228  
 C -0.30042 -4.34148 4.77782  
 C -1.74059 -4.19909 4.69740  
 C -2.60749 -5.31715 4.53708  
 C -3.80187 -5.19467 3.87770  
 C -4.21439 -3.94513 3.33361  
 C -5.05552 -3.85372 2.15649  
 C -5.52770 -5.00642 1.46621  
 C -5.76256 -4.97286 0.11713  
 C -5.54090 -3.78492 -0.63610  
 C -5.14553 -3.81536 -2.03049  
 C -4.94976 -5.03497 -2.73876  
 C -4.04450 -5.11792 -3.76333  
 C -3.27054 -3.98716 -4.15100  
 C 7.53088 -1.30896 -0.62089  
 C 7.55504 0.09312 -0.03311  
 O 7.58332 0.30879 1.17244  
 C 7.58538 -2.38848 0.44904  
 N 7.55084 1.09500 -0.94676  
 H -4.74413 6.94501 -0.14066  
 H -4.08977 6.89588 -2.45577  
 H -2.70827 6.76784 -4.03144  
 H -0.49539 6.55556 -4.95812  
 H 1.58796 6.35007 -4.83663  
 H 3.68770 6.13362 -3.67685  
 H 4.92298 5.99639 -1.98341  
 H 5.33568 5.93650 0.38901  
 H 4.73799 5.98867 2.40023  
 H 3.14735 6.13550 4.20196

H 1.22478 6.31988 5.01532  
 H -1.16831 6.55615 4.89199  
 H -2.99903 6.74338 3.88537  
 H -4.39195 6.89436 1.92721  
 H -1.92391 -6.27395 -5.01409  
 H 0.46901 -6.51191 -4.89039  
 H 2.29719 -6.70039 -3.87824  
 H 3.68913 -6.85060 -1.91973  
 H 4.05223 -6.89963 0.14751  
 H 3.39977 -6.85047 2.46308  
 H 2.01521 -6.72294 4.03836  
 H -0.19853 -6.51068 4.96305  
 H -2.28198 -6.30506 4.84230  
 H -4.38094 -6.08971 3.68085  
 H -5.60483 -5.95633 1.98296  
 H -6.01714 -5.89695 -0.38929  
 H -5.43884 -5.94246 -2.40342  
 H -3.84825 -6.08796 -4.20560  
 H 7.45747 -3.37738 0.00243  
 H 6.79508 -2.23840 1.18883  
 H 8.54209 -2.36540 0.97622  
 H 8.36929 -1.40383 -1.32025  
 H 6.62087 -1.40171 -1.22740  
 H 7.43629 0.91397 -1.93143  
 H 7.47505 2.04736 -0.62163

Propanoic acid-concave  
surface of SWCNT, CPCM

C 4.37947 -0.20090 4.77502  
 C 4.35212 -1.62691 4.51640  
 C 3.12204 -2.23446 4.19618  
 C 1.89119 -1.54983 4.46471  
 C 1.91837 -0.16785 4.71211  
 C 3.17392 0.52433 4.69631  
 C 5.53681 -2.37499 4.26200  
 C 5.51253 -3.47865 3.45166  
 C 4.30130 -3.91194 2.84077  
 C 3.09632 -3.38944 3.35165  
 C 1.84020 -3.81762 2.80826  
 C 1.82093 -4.46467 1.56192  
 C 3.05588 -4.69010 0.86847  
 C 4.28047 -4.58616 1.55784  
 C 0.61717 -3.35067 3.37626  
 C 0.64321 -2.19468 4.21376  
 C 0.57758 -4.63972 0.88339  
 C -0.63312 -4.44212 1.57686  
 C -0.61264 -3.78505 2.84376  
 C -1.83658 -3.28205 3.37869  
 C -1.81114 -2.14516 4.20273  
 C -0.56180 -1.51972 4.49207  
 C -0.53497 -0.11531 4.74534  
 C 0.69630 0.56839 4.70757  
 C -1.87528 -4.59029 0.88918  
 C -3.11145 -4.40844 1.59258  
 C -3.09195 -3.73927 2.85752  
 C -4.29846 -3.29371 3.43392  
 C -4.27180 -2.12339 4.28833  
 C -3.04059 -1.47434 4.50881  
 C -3.01324 -0.06769 4.77002  
 C -1.75740 0.62049 4.70979  
 C -4.33701 -4.62766 0.93283  
 C -5.52857 -4.46560 1.69511  
 C -5.51034 -3.81978 2.90291  
 C -4.21723 0.66353 4.81087  
 C -5.42920 -0.07725 4.90961  
 C -5.45561 -1.42315 4.65654  
 C -1.73578 1.97765 4.35124  
 C -2.96996 2.64361 4.05379  
 C -4.19445 2.06527 4.44299  
 C 0.71848 1.94780 4.34084  
 C -0.49202 2.59617 4.02484  
 C -0.48078 3.68455 3.10181  
 C -1.71401 4.12220 2.53210  
 C -2.95885 3.73479 3.12831  
 C -4.17273 4.22631 2.60793

C -5.37243 3.84000 3.27068  
 C -5.38274 2.79617 4.15730  
 C -1.71598 4.69331 1.24991  
 C -2.96329 4.87182 0.56584  
 C -4.17491 4.81346 1.28291  
 C 0.74073 4.08631 2.52590  
 C 0.73887 4.66731 1.22209  
 C -0.48447 4.82439 0.54014  
 C -0.49923 4.77043 -0.88653  
 C -1.74491 4.58563 -1.55839  
 C -2.97809 4.81546 -0.86435  
 C -4.20422 4.70150 -1.54927  
 C -5.39138 4.98383 -0.81495  
 C -5.37716 5.03849 0.55345  
 C -1.76781 3.91985 -2.79426  
 C -3.02384 3.48530 -3.33181  
 C -4.22800 4.01338 -2.82469  
 C 0.71015 4.56355 -1.57983  
 C 0.68681 3.88799 -2.83745  
 C -0.54552 3.44158 -3.35522  
 C -0.57266 2.26250 -4.19188  
 C -1.82100 1.64126 -4.44283  
 C -3.05077 2.32567 -4.17014  
 C -4.28115 1.71729 -4.48742  
 C -5.46575 2.46511 -4.23210  
 C -5.44037 3.57390 -3.42878  
 C -1.84591 0.26104 -4.69907  
 C -3.10033 -0.43191 -4.68410  
 C -4.30708 0.29274 -4.75285  
 C 0.63299 1.61642 -4.48305  
 C 0.60734 0.21314 -4.74401  
 C -0.62240 -0.47357 -4.70507  
 C -0.64048 -1.85531 -4.34844  
 C -1.88197 -2.46349 -3.99636  
 C -3.11838 -1.81783 -4.32753  
 C -4.34383 -2.45226 -4.04275  
 C -5.53639 -1.78008 -4.43486  
 C -5.51873 -0.45446 -4.77759  
 C -1.88993 -3.53954 -3.09499  
 C -3.13574 -3.96481 -2.52598  
 C -4.35254 -3.56201 -3.11109  
 C 0.57147 -2.50344 -4.03976  
 C 0.56294 -3.59271 -3.11862  
 C -0.65672 -3.99690 -2.54296  
 C -0.65552 -4.55521 -1.23036  
 C -1.88638 -4.64904 -0.51435  
 C -3.13421 -4.53033 -1.21092  
 C -4.34832 -4.69324 -0.51495  
 C -5.55295 -4.59834 -1.26927  
 C -5.55498 -4.04943 -2.52342  
 C 0.56599 -4.69621 -0.54256  
 C 3.04403 -4.74171 -0.56192  
 C 1.79833 -4.56789 -1.24982  
 C 1.79635 -4.01289 -2.53828  
 C 3.04170 -3.62393 -3.13221  
 C 3.05013 -2.53803 -4.06367  
 C 1.81279 -1.87809 -4.36241  
 C 1.83133 -0.51954 -4.71647  
 C 3.08505 0.17324 -4.77907  
 C 3.11084 1.58009 -4.51607  
 C 1.88157 2.24687 -4.20047  
 C 1.90859 3.38304 -3.37555  
 C 3.16514 3.84791 -2.86545  
 C 3.18882 4.52253 -1.60339  
 C 1.95512 4.71105 -0.89757  
 C 1.96954 4.76248 0.50549  
 C 3.21730 4.62419 1.19832  
 C 3.21904 4.04237 2.50569  
 C 1.97289 3.61980 3.07458  
 C 1.96169 2.55052 3.98405  
 C 3.19635 1.90635 4.32447  
 C 5.46898 -4.86418 0.82441  
 C 5.45774 -4.91198 -0.54449  
 C 4.25747 -4.68583 -1.27640  
 C 4.25654 -4.10529 -2.60433

C 5.45635 -3.71682 -3.26547  
 C 5.46405 -2.67867 -4.15892  
 C 4.27286 -1.95546 -4.45219  
 C 4.29094 -0.55449 -4.82385  
 C 5.50052 0.18957 -4.92822  
 C 5.52494 1.53569 -4.67593  
 C 4.34115 2.23289 -4.30155  
 C 4.36928 3.40359 -3.44710  
 C 5.58287 3.93145 -2.92096  
 C 5.60551 4.57578 -1.71238  
 C 4.41638 4.73798 -0.94607  
 C 4.43121 4.79086 0.50277  
 C 5.63555 4.68380 1.25555  
 C 5.63706 4.12759 2.50722  
 C 4.43451 3.64014 3.09406  
 C 4.42275 2.53710 4.03475  
 C 5.61312 1.86704 4.43667  
 C 5.59205 0.54526 4.79459  
 H -6.34436 5.05248 -1.32713  
 H -6.31946 5.14805 1.07796  
 H -6.31560 4.30061 2.99959  
 H -6.33363 2.46448 4.55844  
 H -6.36815 0.43621 5.08206  
 H -6.41400 -1.92944 4.63598  
 H -6.45285 -3.61977 3.39970  
 H -6.48511 -4.75664 1.27638  
 H -6.50153 -4.85965 -0.81402  
 H -6.50567 -3.89275 -3.02016  
 H -6.49301 -2.28489 -4.36265  
 H -6.46195 0.04538 -4.96630  
 H -6.42364 2.10200 -4.58653  
 H -6.37921 4.05185 -3.17318  
 H 6.57099 2.36895 4.36086  
 H 6.53408 0.04583 4.99038  
 H 6.49408 -2.01425 4.62056  
 H 6.45157 -3.95563 3.19502  
 H 6.42079 -4.93634 1.33825  
 H 6.40124 -5.02035 -1.06719  
 H 6.40130 -4.16974 -2.98747  
 H 6.41472 -2.34363 -4.55781  
 H 6.43977 -0.32172 -5.10570  
 H 6.48211 2.04451 -4.66103  
 H 6.52367 3.73255 -3.42147  
 H 6.56358 4.86589 -1.29639  
 H 6.58502 4.94354 0.80115  
 H 6.58803 3.96664 3.00209  
 C -2.62493 -0.76086 -0.69143  
 C -1.69163 -0.89978 0.50249  
 H -3.63357 -0.50509 -0.36059  
 H -2.27440 0.01754 -1.37611  
 H -2.67054 -1.69779 -1.25226  
 H -1.64191 0.02049 1.09685  
 H -2.03425 -1.68025 1.19386  
 C -0.28269 -1.24796 0.09218  
 O 0.54143 -1.32794 1.15152  
 O 0.09701 -1.42817 -1.04208  
 H 1.42243 -1.57213 0.82325

Propanoic acid-graphene,  
CPCM

C 3.70468 5.62708 -0.17472  
 C 2.96293 4.43675 -0.18984  
 C 3.65667 3.20049 -0.18756  
 C 5.08137 3.19424 -0.16792  
 C 5.80089 4.41987 -0.15217  
 C 5.08882 5.62020 -0.15607  
 C 5.78903 1.96386 -0.16555  
 C 7.22941 1.96578 -0.14713  
 C 7.92339 3.23186 -0.13099  
 C 7.24215 4.39845 -0.13322  
 C 2.94191 1.96269 -0.20372  
 C 3.64882 0.74403 -0.20074  
 C 5.08121 0.74444 -0.17979  
 C 5.79246 -0.48470 -0.17652  
 C 7.22965 -0.47241 -0.15970

C 7.91225 0.77166 -0.14537  
 C 2.94601 -0.49893 -0.21085  
 C 3.65731 -1.71484 -0.20422  
 C 5.09534 -1.71186 -0.18756  
 C 5.81824 -2.93229 -0.18314  
 C 7.25015 -2.90861 -0.16909  
 C 7.92333 -1.67933 -0.15746  
 C 5.13525 -4.18474 -0.19203  
 C 3.66983 -4.18569 -0.20256  
 C 2.95487 -2.95661 -0.20764  
 C 1.52678 -2.95841 -0.21635  
 C 0.80813 -1.72273 -0.23322  
 C 1.51271 -0.50004 -0.23626  
 C 0.80336 0.73922 -0.24580  
 C 1.50880 1.96147 -0.23096  
 C 0.79822 3.19988 -0.23545  
 C 1.50536 4.43222 -0.21170  
 C 5.88490 -5.35418 -0.18825  
 C 7.29176 -5.32792 -0.17611  
 C 7.96673 -4.13411 -0.16639  
 C 0.82294 -4.18998 -0.20843  
 C 1.55775 -5.37745 -0.21119  
 C 2.94058 -5.37440 -0.20876  
 C -0.62844 0.73718 -0.27807  
 C -1.33414 -0.50379 -0.26795  
 C -0.62663 -1.72447 -0.25263  
 C -1.34177 -2.96211 -0.23267  
 C -0.63490 -4.19161 -0.20188  
 C -0.63062 3.19793 -0.26873  
 C -1.33828 1.95756 -0.28774  
 C -2.76762 -0.50583 -0.28067  
 C -3.47556 -1.72393 -0.26517  
 C -2.76995 -2.96413 -0.24085  
 C -3.48180 -4.19480 -0.21637  
 C -2.74963 -5.38077 -0.16890  
 C -1.36681 -5.38020 -0.16126  
 C -3.47382 0.73450 -0.29820  
 C -2.77099 1.95482 -0.30493  
 C -4.90586 0.73071 -0.31190  
 C -5.61414 -0.50027 -0.30182  
 C -4.91384 -1.72530 -0.27710  
 C -5.63338 -2.94766 -0.26548  
 C -4.94708 -4.19807 -0.23838  
 C -1.34198 4.42901 -0.27146  
 C -0.61030 5.61924 -0.23625  
 C 0.77000 5.62067 -0.20848  
 C -2.79913 4.42894 -0.30828  
 C -3.48880 3.19031 -0.31577  
 C -4.91352 3.18024 -0.33636  
 C -5.61751 1.94795 -0.33307  
 C -7.05789 1.94572 -0.35066  
 C -7.73751 0.74981 -0.34316  
 C -7.05139 -0.49216 -0.31767  
 C -7.74181 -1.70089 -0.30857  
 C -7.06533 -2.92814 -0.28324  
 C -7.77848 -4.15564 -0.27597  
 C -7.10026 -5.34742 -0.25484  
 C -5.69335 -5.36963 -0.23709  
 C -5.63650 4.40378 -0.35752  
 C -7.07765 4.37824 -0.37868  
 C -7.75551 3.20965 -0.37522  
 C -4.92797 5.60625 -0.35848  
 C -3.54399 5.61718 -0.33374  
 C -0.43884 -0.46083 3.06955  
 C -1.11349 0.86268 2.81950  
 C -1.43039 -1.60984 3.16746  
 H -7.60540 5.32730 -0.39713  
 H 7.76724 5.34909 -0.12068  
 H -8.82851 -1.69453 -0.32147  
 H -8.82429 0.74612 -0.35585  
 H -8.84117 3.19355 -0.39028  
 H -8.86382 -4.12951 -0.28916  
 H -7.64388 -6.28618 -0.25211  
 H -5.20338 -6.33528 -0.22435  
 H -3.25487 -6.33777 -0.13373

|   |          |          |          |
|---|----------|----------|----------|
| H | -0.86355 | -6.33732 | -0.11825 |
| H | 1.05660  | -6.33658 | -0.21971 |
| H | 3.44821  | -6.33076 | -0.21126 |
| H | 5.39767  | -6.32129 | -0.19447 |
| H | 7.83800  | -6.26515 | -0.17392 |
| H | 9.05202  | -4.10489 | -0.15628 |
| H | 9.01002  | -1.66991 | -0.14592 |
| H | 8.99902  | 0.77107  | -0.13230 |
| H | 9.00909  | 3.21896  | -0.11687 |
| H | -5.47511 | 6.54406  | -0.37831 |
| H | -3.04403 | 6.57732  | -0.33679 |
| H | -1.11623 | 6.57599  | -0.22795 |
| H | 1.27284  | 6.57872  | -0.18139 |
| H | 3.20223  | 6.58589  | -0.17931 |
| H | 5.63334  | 6.55968  | -0.14479 |
| H | -2.07066 | -1.49726 | 4.04551  |
| H | -2.07584 | -1.63920 | 2.28576  |
| H | -0.90314 | -2.56339 | 3.24275  |
| H | 0.15600  | -0.35860 | 3.98384  |
| H | 0.28409  | -0.61286 | 2.25957  |
| O | -0.22368 | 1.86570  | 2.71834  |
| O | -2.30592 | 1.03857  | 2.71628  |
| H | -0.71848 | 2.67965  | 2.52868  |

Propanoic acid-convex  
surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -0.78916 | -4.38263 | -4.64869 |
| C | 0.37869  | -4.94415 | -3.99872 |
| C | 1.35762  | -4.06796 | -3.48892 |
| C | 1.37994  | -2.69683 | -3.90788 |
| C | 0.24856  | -2.15285 | -4.53664 |
| C | -0.90273 | -2.98143 | -4.74563 |
| C | 0.43491  | -6.30300 | -3.57620 |
| C | 1.18537  | -6.67418 | -2.49243 |
| C | 1.93146  | -5.71244 | -1.75320 |
| C | 2.14181  | -4.45569 | -2.35584 |
| C | 2.91849  | -3.45805 | -1.67982 |
| C | 3.16565  | -3.59820 | -0.30427 |
| C | 2.63889  | -4.73633 | 0.39084  |
| C | 2.18907  | -5.85781 | -0.33400 |
| C | 3.19332  | -2.21090 | -2.31801 |
| C | 2.41270  | -1.82504 | -3.44954 |
| C | 3.68277  | -2.48907 | 0.42947  |
| C | 4.22025  | -1.38138 | -0.25749 |
| C | 3.97155  | -1.24040 | -1.65636 |
| C | 4.21751  | 0.01920  | -2.27908 |
| C | 3.45258  | 0.39808  | -3.39334 |
| C | 2.44227  | -0.48380 | -3.88146 |
| C | 1.29244  | 0.06916  | -4.52177 |
| C | 0.15303  | -0.73900 | -4.70747 |
| C | 4.71454  | -0.26220 | 0.47578  |
| C | 5.27853  | 0.85884  | -0.21782 |
| C | 5.02586  | 1.00160  | -1.61838 |
| C | 5.33297  | 2.21392  | -2.26766 |
| C | 4.54257  | 2.60585  | -3.41794 |
| C | 3.50143  | 1.75794  | -3.84561 |
| C | 2.34986  | 2.31164  | -4.48935 |
| C | 1.18923  | 1.48623  | -4.65749 |
| C | 5.83988  | 1.92650  | 0.50895  |
| C | 6.42943  | 2.98540  | -0.23827 |
| C | 6.18390  | 3.12472  | -1.57933 |
| C | 2.26112  | 3.70278  | -4.69468 |
| C | 3.45685  | 4.46248  | -4.55104 |
| C | 4.55893  | 3.93266  | -3.93378 |
| C | -0.08026 | 2.08533  | -4.68136 |
| C | -0.18621 | 3.50799  | -4.53855 |
| C | 0.95002  | 4.32102  | -4.72065 |
| C | -1.13795 | -0.12974 | -4.73191 |
| C | -1.24387 | 1.26609  | -4.56987 |
| C | -2.42104 | 1.81216  | -3.97477 |
| C | -2.39938 | 3.16080  | -3.50797 |
| C | -1.36606 | 4.05513  | -3.94153 |
| C | -1.38702 | 5.40483  | -3.53665 |
| C | -0.35678 | 6.25264  | -4.03386 |
| C | 0.77191  | 5.72914  | -4.60632 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -3.21590 | 3.52951  | -2.42677 |
| C | -2.99724 | 4.79106  | -1.78169 |
| C | -2.22982 | 5.78517  | -2.42045 |
| C | -3.45104 | 0.94315  | -3.56231 |
| C | -4.28144 | 1.31828  | -2.46335 |
| C | -4.05296 | 2.54863  | -1.81527 |
| C | -4.37265 | 2.67705  | -0.42979 |
| C | -3.84519 | 3.78245  | 0.30282  |
| C | -3.31703 | 4.91953  | -0.39263 |
| C | -2.86388 | 6.04029  | 0.33129  |
| C | -2.39112 | 7.15505  | -0.41846 |
| C | -2.08454 | 7.03170  | -1.74773 |
| C | -3.59427 | 3.64164  | 1.67704  |
| C | -2.81531 | 4.63810  | 2.35237  |
| C | -2.60420 | 5.89474  | 1.75007  |
| C | -4.91025 | 1.57115  | 0.25853  |
| C | -4.65551 | 1.42823  | 1.65597  |
| C | -3.87140 | 2.39569  | 2.31557  |
| C | -3.09073 | 2.00882  | 3.44659  |
| C | -2.05715 | 2.87932  | 3.90549  |
| C | -2.03265 | 4.25027  | 3.48613  |
| C | -1.05399 | 5.12598  | 3.99733  |
| C | -1.10797 | 6.48446  | 3.57374  |
| C | -1.85712 | 6.85577  | 2.48898  |
| C | -0.92755 | 2.33464  | 4.53671  |
| C | 0.22398  | 3.16240  | 4.74812  |
| C | 0.11183  | 4.56367  | 4.65044  |
| C | -3.12250 | 0.66776  | 3.87863  |
| C | -1.97369 | 0.11378  | 4.51985  |
| C | -0.83379 | 0.92084  | 4.70780  |
| C | 0.45672  | 0.31053  | 4.73480  |
| C | 1.61491  | 1.13231  | 4.59088  |
| C | 1.51757  | 2.55065  | 4.77550  |
| C | 2.67504  | 3.35161  | 4.70432  |
| C | 2.51917  | 4.74684  | 4.94050  |
| C | 1.28102  | 5.33246  | 4.91511  |
| C | 2.77322  | 0.59481  | 4.00724  |
| C | 3.83157  | 1.47681  | 3.60914  |
| C | 3.87111  | 2.79661  | 4.10140  |
| C | 0.56136  | -1.08538 | 4.57191  |
| C | 1.73844  | -1.63175 | 3.97749  |
| C | 2.76994  | -0.76313 | 3.56805  |
| C | 3.59825  | -1.13628 | 2.46689  |
| C | 4.40780  | -0.14165 | 1.84088  |
| C | 4.66345  | 1.10188  | 2.50686  |
| C | 5.52041  | 2.05309  | 1.91783  |
| C | 5.76698  | 3.25024  | 2.64779  |
| C | 4.96995  | 3.60975  | 3.70253  |
| C | 3.36503  | -2.36390 | 1.81483  |
| C | 2.31464  | -4.60792 | 1.77915  |
| C | 2.53069  | -3.34698 | 2.42566  |
| C | 1.71525  | -2.97969 | 3.50789  |
| C | 0.68108  | -3.87383 | 3.93884  |
| C | -0.49863 | -3.32629 | 4.53592  |
| C | -0.60318 | -1.90376 | 4.68067  |
| C | -1.87204 | -1.30340 | 4.65550  |
| C | -3.03357 | -2.12716 | 4.48698  |
| C | -4.18538 | -1.57144 | 3.84481  |
| C | -4.13555 | -0.21201 | 3.39219  |
| C | -4.90329 | 0.16858  | 2.27964  |
| C | -5.71794 | -0.81112 | 1.62240  |
| C | -5.97297 | -0.66810 | 0.22134  |
| C | -5.40477 | 0.45017  | -0.47331 |
| C | -5.08989 | 0.32355  | -1.83570 |
| C | -5.34298 | -0.92142 | -2.49983 |
| C | -4.51007 | -1.29784 | -3.60091 |
| C | -3.45283 | -0.41544 | -4.00007 |
| C | -2.29508 | -0.95243 | -4.58516 |
| C | -2.19687 | -2.37059 | -4.76988 |
| C | 1.71532  | -6.97291 | 0.41495  |
| C | 1.40420  | -6.84937 | 1.74310  |
| C | 1.54612  | -5.60248 | 2.41607  |
| C | 0.70114  | -5.22271 | 3.53080  |
| C | -0.33115 | -6.07019 | 4.02458  |
| C | -1.45956 | -5.54646 | 4.59730  |

|   |          |          |          |
|---|----------|----------|----------|
| C | -1.63596 | -4.13829 | 4.71545  |
| C | -2.94622 | -3.51851 | 4.69140  |
| C | -4.14344 | -4.27650 | 4.55006  |
| C | -5.24578 | -3.74480 | 3.93532  |
| C | -5.22839 | -2.41787 | 3.41905  |
| C | -6.02061 | -2.02489 | 2.27082  |
| C | -6.86848 | -2.93924 | 1.58322  |
| C | -7.11265 | -2.80244 | 0.24246  |
| C | -6.52604 | -1.74145 | -0.50486 |
| C | -6.20057 | -1.87228 | -1.91147 |
| C | -6.44580 | -3.07081 | -2.64008 |
| C | -5.64775 | -3.43142 | -3.69335 |
| C | -4.54908 | -2.61793 | -4.09238 |
| C | -3.35352 | -3.17243 | -4.69628 |
| C | -3.19708 | -4.56764 | -4.93275 |
| C | -1.95850 | -5.15234 | -4.91044 |
| H | -2.16667 | 8.09035  | 0.08150  |
| H | -1.62586 | 7.87272  | -2.25519 |
| H | -0.40623 | 7.32261  | -3.86724 |
| H | 1.57835  | 6.40191  | -4.87474 |
| H | 3.47290  | 5.50917  | -4.83267 |
| H | 5.40975  | 4.57772  | -3.74536 |
| H | 6.56349  | 4.00343  | -2.08831 |
| H | 6.99527  | 3.75876  | 0.26837  |
| H | 6.52304  | 3.94847  | 2.30711  |
| H | 5.12280  | 4.57995  | 4.16136  |
| H | 3.39182  | 5.38269  | 5.03692  |
| H | 1.21567  | 6.41175  | 4.99358  |
| H | -0.46964 | 7.22555  | 4.04094  |
| H | -1.78628 | 7.87772  | 2.13460  |
| H | -4.06947 | -5.20414 | -5.02716 |
| H | -1.89252 | -6.23158 | -4.98921 |
| H | -0.20285 | -7.04456 | -4.04344 |
| H | 1.11605  | -7.69641 | -2.13865 |
| H | 1.49377  | -7.90878 | -0.08523 |
| H | 0.94537  | -7.69094 | 2.24952  |
| H | -0.28334 | -7.13978 | 3.85511  |
| H | -2.26727 | -6.21881 | 4.86293  |
| H | -4.16080 | -5.32293 | 4.83261  |
| H | -6.09849 | -4.38817 | 3.74985  |
| H | -7.24446 | -3.81921 | 2.09262  |
| H | -7.67347 | -3.57906 | -0.26476 |
| H | -7.20286 | -3.76821 | -2.29998 |
| H | -5.80022 | -4.40185 | -4.15181 |
| H | 6.57820  | -4.33535 | 1.45389  |
| C | 6.93649  | -3.30946 | 1.34677  |
| H | 6.19163  | -2.63573 | 1.78041  |
| H | 7.85979  | -3.19822 | 1.91886  |
| C | 7.17001  | -2.97415 | -0.11929 |
| C | 7.56847  | -1.53227 | -0.30359 |
| H | 7.97521  | -3.58547 | -0.54397 |
| H | 6.28451  | -3.16611 | -0.73252 |
| O | 7.41499  | -1.12239 | -1.57354 |
| O | 7.99007  | -0.80531 | 0.56664  |
| H | 7.69183  | -0.19224 | -1.61713 |

Formic acid-concave  
surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.51950 | 0.21511  | -4.83143 |
| C | -4.31906 | -0.54472 | -4.73515 |
| C | -3.10300 | 0.16684  | -4.71620 |
| C | -3.10429 | 1.57758  | -4.47420 |
| C | -4.32197 | 2.25073  | -4.25198 |
| C | -5.52080 | 1.56474  | -4.59758 |
| C | -1.85857 | -0.54243 | -4.66011 |
| C | -1.85556 | -1.89560 | -4.28680 |
| C | -3.09680 | -2.53950 | -3.97269 |
| C | -4.31557 | -1.94299 | -4.35318 |
| C | -3.09299 | -3.62791 | -3.04389 |
| C | -4.30966 | -4.09619 | -2.50884 |
| C | -5.50995 | -3.69193 | -3.15939 |
| C | -5.51269 | -2.65217 | -4.05086 |
| C | -1.84867 | -4.03900 | -2.46279 |
| C | -0.61528 | -3.62075 | -3.04534 |
| C | -0.61883 | -2.53346 | -3.97020 |

C 0.59885 -1.90752 -4.30572  
 C 0.59594 -0.53086 -4.68557  
 C -0.62467 0.17227 -4.71713  
 C -0.62594 1.57949 -4.47768  
 C -1.86139 2.23136 -4.18648  
 C -1.84511 -4.60736 -1.17960  
 C -3.08742 -4.75054 -0.47836  
 C -4.30684 -4.67482 -1.18044  
 C 0.60676 -4.04139 -2.48231  
 C 0.61110 -4.62114 -1.17724  
 C -0.60774 -4.75470 -0.48217  
 C -0.60339 -4.67574 0.94422  
 C -1.83871 -4.45278 1.62594  
 C -3.08467 -4.67234 0.95077  
 C -4.29955 -4.52764 1.64945  
 C -5.50044 -4.79852 0.93372  
 C -5.50395 -4.86918 -0.43392  
 C 1.84034 -3.59315 -3.04448  
 C 1.83662 -2.52742 -3.95819  
 C 0.61677 -4.48084 1.62229  
 C 1.85068 -4.66114 0.92917  
 C 1.84784 -4.72887 -0.47270  
 C 3.08935 -4.61137 -1.17999  
 C 3.08604 -4.03412 -2.48890  
 C 4.30074 -3.65534 -3.09374  
 C 4.29669 -2.55580 -4.03844  
 C 3.07794 -1.90625 -4.31762  
 C 3.07457 -0.52704 -4.69924  
 C 1.83030 0.18488 -4.70886  
 C 1.82892 1.56897 -4.47290  
 C 0.59346 2.23442 -4.21341  
 C 3.09503 -4.47843 1.61680  
 C 4.31180 -4.72262 0.94968  
 C 4.30882 -4.79223 -0.49797  
 C 5.50573 -4.71107 -1.26576  
 C 5.50185 -4.16166 -2.52023  
 C 4.29061 0.17843 -4.79525  
 C 5.49060 -0.58757 -4.82119  
 C 5.49357 -1.90752 -4.45619  
 C 4.28908 1.60754 -4.55127  
 C 3.07212 2.23885 -4.22649  
 C 0.59437 3.40212 -3.39190  
 C 1.83093 3.86805 -2.85255  
 C 3.07302 3.40874 -3.40196  
 C 4.29136 3.92324 -2.91540  
 C 5.48897 3.45921 -3.53055  
 C 5.48769 2.34073 -4.32087  
 C -1.86061 3.37938 -3.37772  
 C -0.62421 3.87242 -2.86235  
 C -0.62106 4.56140 -1.61178  
 C 0.60036 4.75502 -0.93589  
 C 1.83395 4.54485 -1.62225  
 C 3.07942 4.76029 -0.94565  
 C 4.29451 4.62194 -1.64537  
 C 0.60503 4.82225 0.49051  
 C 1.84298 4.67573 1.18592  
 C 3.08414 4.82716 0.48425  
 C 4.30381 4.75325 1.18602  
 C 5.49999 4.95361 0.43952  
 C 5.49548 4.88995 -0.92852  
 C -3.10315 3.86928 -2.85673  
 C -3.10018 4.55996 -1.60315  
 C -1.85457 4.73622 -0.91538  
 C -1.84994 4.80263 0.48711  
 C -0.61202 4.69275 1.18926  
 C -0.60731 4.12451 2.49869  
 C 0.61433 3.70641 3.06318  
 C 1.84763 4.11635 2.47342  
 C 3.09325 3.71071 3.05619  
 C 4.30872 4.17538 2.51530  
 C 0.61804 2.62618 3.99626  
 C 1.85483 1.98749 4.31134  
 C 3.09697 2.62778 3.99154  
 C 4.31565 2.02919 4.36880  
 C 5.51336 2.73424 4.05905

C 5.51009 3.77083 3.16375  
 C -3.09095 4.69383 1.19694  
 C -3.08626 4.12510 2.50997  
 C -1.84066 3.68536 3.06716  
 C -1.83703 2.62349 3.98526  
 C -0.60001 2.00197 4.33192  
 C -0.59800 0.62443 4.70629  
 C 0.62195 -0.08019 4.73319  
 C 1.85673 0.63291 4.68001  
 C 3.10013 -0.07866 4.73115  
 C 4.31735 0.63092 4.75136  
 C 0.62204 -1.48557 4.48312  
 C 1.85616 -2.13914 4.19077  
 C 3.09955 -1.48848 4.48352  
 C 4.31640 -2.16348 4.26270  
 C 5.51592 -1.48018 4.61122  
 C 5.51658 -0.13085 4.84686  
 C -3.07890 2.00303 4.34377  
 C -3.07679 0.62207 4.71991  
 C -1.83286 -0.09055 4.72510  
 C -1.83257 -1.47282 4.47905  
 C -0.59765 -2.13750 4.21506  
 C -0.59836 -3.30378 3.39178  
 C 0.61907 -3.78042 2.86617  
 C 1.85455 -3.28701 3.38184  
 C 3.09710 -3.78126 2.86642  
 C 4.31502 -3.34802 3.42752  
 C 5.51242 -4.56826 1.69957  
 C 5.51388 -3.90494 2.89783  
 C -3.07628 -2.14053 4.22977  
 C -3.07821 -3.30767 3.40174  
 C -1.83605 -3.76679 2.85171  
 C -4.29636 -3.82348 2.91659  
 C -5.49367 -3.35922 3.53192  
 C -5.49168 -2.24241 4.32475  
 C -4.29289 -1.51064 4.55849  
 C -4.29339 -0.08310 4.81137  
 C -5.49302 0.68348 4.84118  
 C -5.49498 2.00456 4.48055  
 C -4.29754 2.65290 4.06407  
 C -4.30121 3.75019 3.11685  
 C -5.50221 4.25492 2.54145  
 C -5.50683 4.79850 1.28442  
 C -4.31060 4.87448 0.51495  
 C -4.31561 4.80263 -0.93298  
 C -5.51717 4.64843 -1.68150  
 C -5.52000 3.98777 -2.88134  
 C -4.32143 3.43473 -3.41582  
 O 1.06795 -1.65480 0.33543  
 C 0.28225 -1.48764 -0.56211  
 O -1.03937 -1.63623 -0.45299  
 H 0.54755 -1.18783 -1.58701  
 H 6.45063 5.05175 0.95113  
 H 6.44256 4.93911 -1.45376  
 H 6.43797 3.92616 -3.29276  
 H 6.43556 1.95958 -4.68325  
 H 6.43864 -0.10433 -5.02844  
 H 6.44384 -2.24255 -4.38734  
 H 6.44917 -4.02066 -3.02789  
 H 6.45573 -4.98565 -0.82129  
 H 6.46078 -4.88043 1.27719  
 H 6.46324 -3.71438 3.38526  
 H 6.46463 -2.00428 4.58936  
 H 6.46624 0.36745 5.00465  
 H 6.46379 2.38702 4.44793  
 H 6.45813 4.20972 2.87413  
 H -6.47037 2.08727 -4.57495  
 H -6.46860 -0.28475 -4.98743  
 H -6.46235 -2.30662 -4.44307  
 H -6.45767 -4.13488 -2.87492  
 H -6.45447 -4.96679 -0.94586  
 H -6.44789 -4.84317 1.45864  
 H -6.44292 -3.82528 3.29354  
 H -6.43948 -1.86179 4.68789  
 H -6.44133 0.20014 5.04693

H -6.44487 2.52251 4.41305  
 H -6.44930 4.11738 3.05055  
 H -6.45693 5.07270 0.83996  
 H -6.46529 4.95816 -1.25684  
 H -6.47020 3.79637 -3.36682  
 H -1.23284 -1.92078 0.45860

# Formic acid-graphene, CPCM

C 7.80040 -3.14757 -0.23240  
 C 7.09832 -1.88608 -0.20915  
 C 5.65787 -1.89302 -0.20458  
 C 4.95810 -3.12758 -0.22050  
 C 5.68533 -4.34863 -0.24182  
 C 7.12650 -4.31833 -0.24819  
 C 4.98082 -5.55332 -0.25802  
 C 3.59670 -5.56883 -0.24847  
 C 2.84767 -4.38319 -0.22253  
 C 3.53333 -3.14241 -0.21420  
 C 2.81111 -1.90922 -0.20261  
 C 1.37822 -1.91682 -0.20292  
 C 0.67479 -3.15962 -0.19947  
 C 1.39024 -4.38804 -0.20174  
 C 3.50986 -0.68635 -0.18281  
 C 4.94210 -0.67813 -0.18466  
 C 2.79954 0.55179 -0.16693  
 C 1.36635 0.54463 -0.16312  
 C 0.66457 -0.69867 -0.19248  
 C -0.76725 -0.70580 -0.16320  
 C -1.46862 -1.93051 -0.16740  
 C -0.75401 -3.16649 -0.18058  
 C -1.45719 -4.40120 -0.17533  
 C -0.71799 -5.58729 -0.16895  
 C 0.66249 -5.58101 -0.18028  
 C 0.65462 1.76217 -0.13746  
 C -0.78020 1.75522 -0.12040  
 C -1.48038 0.53082 -0.13740  
 C -2.91373 0.52469 -0.11674  
 C -3.61269 -0.72046 -0.12746  
 C -2.90181 -1.93670 -0.14640  
 C -3.61264 -3.17686 -0.15393  
 C -2.91486 -4.41072 -0.17160  
 C -5.03743 -3.17549 -0.14394  
 C -5.74908 -1.94757 -0.12285  
 C -5.04520 -0.72587 -0.11260  
 C -5.76058 0.50076 -0.09072  
 C -5.06740 1.73014 -0.08110  
 C -3.62929 1.73796 -0.09532  
 C -2.93102 2.98193 -0.08539  
 C -1.50297 2.98845 -0.09729  
 C -5.75298 -4.40346 -0.15618  
 C -5.03698 -5.60124 -0.17979  
 C -3.65272 -5.60342 -0.18770  
 C -7.18953 -1.95439 -0.11119  
 C -7.87943 -3.22277 -0.12406  
 C -7.19440 -4.38691 -0.14595  
 C -7.19778 0.48357 -0.07721  
 C -7.87630 -0.76276 -0.08872  
 C -5.79438 2.94799 -0.05775  
 C -7.22620 2.91940 -0.04216  
 C -7.89542 1.68797 -0.05306  
 C -3.65015 4.20857 -0.06717  
 C -5.11548 4.20270 -0.04779  
 C -5.86879 5.36940 -0.01812  
 C -7.27554 5.33829 -0.00252  
 C -7.94667 4.14238 -0.01505  
 C 1.36567 3.00216 -0.11194  
 C 0.65448 4.22932 -0.08358  
 C -0.80341 4.22255 -0.08564  
 C -1.54225 5.40747 -0.07936  
 C -2.92506 5.39971 -0.07056  
 C 2.79362 3.00904 -0.11767  
 C 3.50113 4.24219 -0.09162  
 C 2.76488 5.42593 -0.05295  
 C 1.38207 5.42064 -0.04885

|   |          |          |          |
|---|----------|----------|----------|
| C | 3.50338  | 1.77153  | -0.14220 |
| C | 5.64622  | 0.55506  | -0.16547 |
| C | 4.94159  | 1.77767  | -0.14413 |
| C | 5.65718  | 3.00229  | -0.12506 |
| C | 4.96656  | 4.25039  | -0.10215 |
| C | 7.77389  | -0.68799 | -0.19177 |
| C | 7.08358  | 0.55169  | -0.16920 |
| C | 7.77006  | 1.76253  | -0.15192 |
| C | 7.08932  | 2.98751  | -0.13046 |
| C | 7.79834  | 4.21730  | -0.11500 |
| C | 7.11603  | 5.40681  | -0.09737 |
| C | 5.70896  | 5.42437  | -0.09170 |
| C | 1.02341  | -0.81842 | 2.81678  |
| O | 0.22437  | -1.88605 | 2.78247  |
| O | 2.22714  | -0.85949 | 2.81738  |
| H | 0.42590  | 0.10274  | 2.84285  |
| H | 7.65752  | -5.26558 | -0.26616 |
| H | -7.71647 | -5.33926 | -0.15633 |
| H | 8.85684  | 1.75967  | -0.15549 |
| H | 8.86073  | -0.68079 | -0.19489 |
| H | 8.88609  | -3.12779 | -0.23684 |
| H | 8.88383  | 4.19472  | -0.11872 |
| H | 7.65650  | 6.34735  | -0.08765 |
| H | 5.21578  | 6.38839  | -0.07979 |
| H | 3.26678  | 6.38484  | -0.02205 |
| H | 0.87543  | 6.37626  | -0.01339 |
| H | -1.04451 | 6.36840  | -0.08400 |
| H | -3.43594 | 6.35433  | -0.06702 |
| H | -5.38471 | 6.33802  | -0.00432 |
| H | -7.82471 | 6.27356  | 0.02018  |
| H | -9.03185 | 4.10945  | -0.00328 |
| H | -8.98208 | 1.67483  | -0.04204 |
| H | -8.96311 | -0.76592 | -0.07955 |
| H | -8.96523 | -3.21355 | -0.11616 |
| H | 5.53119  | -6.48924 | -0.27845 |
| H | 3.09995  | -6.53051 | -0.26455 |
| H | 1.17169  | -6.53600 | -0.16933 |
| H | -1.21792 | -6.54707 | -0.14994 |
| H | -3.14708 | -6.56030 | -0.21061 |
| H | -5.57854 | -6.54241 | -0.19275 |
| H | 0.78260  | -2.68067 | 2.72846  |

# Formic acid-convex surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.43845 | 0.99390  | 4.86118  |
| C | -4.13980 | 1.55186  | 4.68721  |
| C | -3.04294 | 0.66921  | 4.74763  |
| C | -3.25744 | -0.74270 | 4.65001  |
| C | -4.56476 | -1.24523 | 4.49493  |
| C | -5.64349 | -0.35701 | 4.76904  |
| C | -1.70771 | 1.17543  | 4.62096  |
| C | -1.50962 | 2.46461  | 4.10035  |
| C | -2.64716 | 3.24356  | 3.70652  |
| C | -3.93525 | 2.88214  | 4.14855  |
| C | -2.49801 | 4.19674  | 2.64890  |
| C | -3.63931 | 4.77042  | 2.05380  |
| C | -4.87651 | 4.63074  | 2.74525  |
| C | -5.01916 | 3.71899  | 3.75737  |
| C | -1.21653 | 4.33584  | 2.02172  |
| C | -0.04839 | 3.81840  | 2.65736  |
| C | -0.19675 | 2.86928  | 3.71346  |
| C | 0.92007  | 2.11124  | 4.11946  |
| C | 0.71860  | 0.80046  | 4.64885  |
| C | -0.59258 | 0.29436  | 4.75286  |
| C | -0.80642 | -1.11384 | 4.65424  |
| C | -2.12935 | -1.59918 | 4.42729  |
| C | -1.15160 | 4.72364  | 0.67356  |
| C | -2.36718 | 4.98061  | -0.04149 |
| C | -3.57081 | 5.17781  | 0.66417  |
| C | 1.21157  | 3.97552  | 2.04534  |
| C | 1.27714  | 4.36641  | 0.67418  |
| C | 0.07966  | 4.58943  | -0.03457 |
| C | 0.05045  | 4.37029  | -1.44412 |
| C | -1.21147 | 4.27674  | -2.10353 |
| C | -2.39841 | 4.75177  | -1.45450 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -3.63236 | 4.72258  | -2.13426 |
| C | -4.76607 | 5.24954  | -1.45215 |
| C | -4.73602 | 5.46994  | -0.10052 |
| C | 2.37566  | 3.42889  | 2.66319  |
| C | 2.22973  | 2.49557  | 3.70227  |
| C | 1.21871  | 3.92634  | -2.09479 |
| C | 2.47493  | 3.99257  | -1.42210 |
| C | 2.50494  | 4.21488  | -0.03550 |
| C | 3.72813  | 4.00609  | 0.68229  |
| C | 3.66194  | 3.60560  | 2.05527  |
| C | 4.81816  | 3.12684  | 2.70292  |
| C | 4.66768  | 2.16273  | 3.77493  |
| C | 3.37091  | 1.74046  | 4.12941  |
| C | 3.16910  | 0.42666  | 4.66059  |
| C | 1.83290  | -0.08616 | 4.74474  |
| C | 1.62251  | -1.47094 | 4.64738  |
| C | 0.29790  | -1.96615 | 4.45426  |
| C | 3.66893  | 3.55986  | -2.08665 |
| C | 4.91826  | 3.69080  | -1.44727 |
| C | 4.94906  | 3.92146  | -0.01620 |
| C | 6.13353  | 3.75414  | 0.75638  |
| C | 6.07021  | 3.37016  | 2.06951  |
| C | 4.26798  | -0.43894 | 4.82760  |
| C | 5.56864  | 0.13841  | 4.77536  |
| C | 5.76187  | 1.39531  | 4.26690  |
| C | 4.05097  | -1.86869 | 4.72668  |
| C | 2.74856  | -2.33966 | 4.46585  |
| C | 0.11295  | -3.19468 | 3.75122  |
| C | 1.25791  | -3.89228 | 3.26211  |
| C | 2.56307  | -3.57146 | 3.76133  |
| C | 3.68326  | -4.31020 | 3.33073  |
| C | 4.94624  | -3.97014 | 3.89317  |
| C | 5.12390  | -2.79121 | 4.56739  |
| C | -2.31126 | -2.80709 | 3.73548  |
| C | -1.16989 | -3.52815 | 3.27262  |
| C | -1.28921 | -4.33786 | 2.10305  |
| C | -0.12193 | -4.78647 | 1.45332  |
| C | 1.14040  | -4.68924 | 2.11231  |
| C | 2.32796  | -5.16420 | 1.46437  |
| C | 3.56172  | -5.13424 | 2.14433  |
| C | -0.15260 | -5.01550 | 0.04426  |
| C | 1.08051  | -5.14056 | -0.66318 |
| C | 2.29698  | -5.39382 | 0.05187  |
| C | 3.50094  | -5.58905 | -0.65339 |
| C | 4.66640  | -5.88041 | 0.11115  |
| C | 4.69600  | -5.66064 | 1.46282  |
| C | -3.62075 | -3.15681 | 3.26825  |
| C | -3.74027 | -3.96774 | 2.09510  |
| C | -2.54645 | -4.40197 | 1.43040  |
| C | -2.57651 | -4.62677 | 0.04470  |
| C | -1.34880 | -4.78774 | -0.66505 |
| C | -1.28190 | -4.38808 | -2.03426 |
| C | -0.02168 | -4.22919 | -2.64514 |
| C | 1.14643  | -4.74700 | -2.00964 |
| C | 2.42815  | -4.60623 | -2.63657 |
| C | 3.56946  | -5.18086 | -2.04276 |
| C | 0.12721  | -3.27826 | -3.69987 |
| C | 1.43993  | -2.87354 | -4.08704 |
| C | 2.57746  | -3.65243 | -3.69341 |
| C | 3.86548  | -3.29144 | -4.13612 |
| C | 4.94922  | -4.12880 | -3.74589 |
| C | 4.80649  | -5.04120 | -2.73436 |
| C | -3.79963 | -4.41588 | -0.67285 |
| C | -3.73261 | -4.01617 | -2.04576 |
| C | -2.44547 | -3.83959 | -2.65210 |
| C | -2.29912 | -2.90526 | -3.69014 |
| C | -0.98939 | -2.52059 | -4.10673 |
| C | -0.78811 | -1.21032 | -4.63748 |
| C | 0.52293  | -0.70412 | -4.74221 |
| C | 1.63803  | -1.58489 | -4.60902 |
| C | 2.97327  | -1.07875 | -4.73632 |
| C | 4.07014  | -1.96128 | -4.67509 |
| C | 0.73663  | 0.70428  | -4.64586 |
| C | 2.05948  | 1.18994  | -4.41916 |
| C | 3.18767  | 0.33325  | -4.64024 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 4.49490  | 0.83608  | -4.48486 |
| C | 5.57377  | -0.05235 | -4.75760 |
| C | 5.36880  | -1.40336 | -4.84894 |
| C | -3.44026 | -2.15079 | -4.11894 |
| C | -3.23863 | -0.83719 | -4.65070 |
| C | -1.90261 | -0.32403 | -4.73480 |
| C | -1.69262 | 1.06092  | -4.63929 |
| C | -0.36799 | 1.55658  | -4.44684 |
| C | -0.18337 | 2.78534  | -3.74445 |
| C | 1.09955  | 3.11891  | -3.26554 |
| C | 2.24121  | 2.39847  | -3.72826 |
| C | 3.55016  | 2.74851  | -3.25990 |
| C | 4.68220  | 2.08462  | -3.77255 |
| C | 6.07128  | 3.28223  | -2.17638 |
| C | 5.95722  | 2.50655  | -3.29935 |
| C | -2.81903 | 1.92935  | -4.45795 |
| C | -2.63391 | 3.16123  | -3.75340 |
| C | -1.32868 | 3.48223  | -3.25499 |
| C | -3.75420 | 3.89904  | -3.32109 |
| C | -5.01741 | 3.55828  | -3.88260 |
| C | -5.19473 | 2.37960  | -4.55740 |
| C | -4.12136 | 1.45775  | -4.71798 |
| C | -4.33776 | 0.02792  | -4.81890 |
| C | -5.63821 | -0.55000 | -4.76800 |
| C | -5.83131 | -1.80693 | -4.25966 |
| C | -4.73723 | -2.57353 | -3.76614 |
| C | -4.88831 | -3.53728 | -2.69401 |
| C | -6.14079 | -3.77932 | -2.06085 |
| C | -6.20474 | -4.16184 | -0.74742 |
| C | -5.02041 | -4.32938 | 0.02537  |
| C | -4.98964 | -4.09848 | 1.45632  |
| C | -6.14245 | -3.68968 | 2.18572  |
| C | -6.02784 | -2.91458 | 3.30894  |
| C | -4.75249 | -2.49316 | 3.78180  |
| O | 1.04076  | 7.57393  | 0.90146  |
| C | 0.93076  | 7.46681  | -0.42336 |
| O | 1.84260  | 7.22137  | -1.17105 |
| H | -0.10888 | 7.63484  | -0.73448 |
| H | 5.58179  | -6.17854 | -0.38734 |
| H | 5.63430  | -5.79375 | 1.98909  |
| H | 5.81196  | -4.59324 | 3.69982  |
| H | 6.12426  | -2.52052 | 4.88546  |
| H | 6.43718  | -0.45374 | 5.04002  |
| H | 6.77657  | 1.75678  | 4.14505  |
| H | 6.99467  | 3.14932  | 2.59078  |
| H | 7.10587  | 3.82567  | 0.28239  |
| H | 7.06154  | 3.49127  | -1.78780 |
| H | 6.86154  | 2.12843  | -3.76228 |
| H | 6.59070  | 0.32164  | -4.78895 |
| H | 6.23011  | -2.05431 | -4.94760 |
| H | 5.93344  | -3.97798 | -4.17453 |
| H | 5.68292  | -5.58197 | -2.39574 |
| H | -6.66039 | -0.73105 | 4.80083  |
| H | -6.29964 | 1.64486  | 4.96082  |
| H | -6.00349 | 3.56800  | 4.18566  |
| H | -5.75313 | 5.17076  | 2.40593  |
| H | -5.65111 | 5.76921  | 0.39785  |
| H | -5.70444 | 5.38332  | -1.97816 |
| H | -5.88352 | 4.18043  | -3.68793 |
| H | -6.19521 | 2.10832  | -4.87458 |
| H | -6.50671 | 0.04163  | -5.03396 |
| H | -6.84591 | -2.16914 | -4.13922 |
| H | -7.06489 | -3.55818 | -2.58260 |
| H | -7.17715 | -4.23216 | -0.27341 |
| H | -7.13283 | -3.89852 | 1.79732  |
| H | -6.93187 | -2.53647 | 3.77242  |
| H | 1.96714  | 7.40116  | 1.14130  |

# Ethylammonium-concave surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -5.61076 | -3.29365 | -3.33942 |
| C | -4.41928 | -3.77770 | -2.72823 |
| C | -3.19219 | -3.32407 | -3.25519 |
| C | -3.16623 | -2.18161 | -4.12101 |
| C | -4.36819 | -1.51910 | -4.44554 |

C -5.58540 -2.20435 -4.16924  
 C -1.95415 -3.80441 -2.70914  
 C -1.95827 -4.43284 -1.45182  
 C -3.20037 -4.58526 -0.74793  
 C -4.42326 -4.43117 -1.43367  
 C -3.18305 -4.60688 0.68547  
 C -4.38963 -4.47477 1.40287  
 C -5.60214 -4.66036 0.68008  
 C -5.61907 -4.63828 -0.68928  
 C -1.92554 -4.47793 1.36528  
 C -0.70453 -4.67777 0.65320  
 C -0.72088 -4.65568 -0.77486  
 C 0.49468 -4.52471 -1.47657  
 C 0.49920 -3.88716 -2.75423  
 C -0.71216 -3.40122 -3.28787  
 C -0.68704 -2.26334 -4.15144  
 C -1.90399 -1.56399 -4.41224  
 C -1.89311 -3.89749 2.64463  
 C -3.11677 -3.43189 3.23074  
 C -4.35521 -3.86645 2.71776  
 C 0.52723 -4.57072 1.32924  
 C 0.56091 -3.98025 2.62834  
 C -0.63760 -3.51749 3.20910  
 C -0.59187 -2.40789 4.10804  
 C -1.80207 -1.71711 4.41745  
 C -3.06989 -2.32363 4.13472  
 C -4.26250 -1.67304 4.50910  
 C -5.48752 -2.34605 4.23780  
 C -5.53297 -3.40536 3.37101  
 C 1.74892 -4.73950 0.61038  
 C 1.73289 -4.71618 -0.79304  
 C 0.65081 -1.81024 4.39971  
 C 1.86223 -2.48014 4.05159  
 C 1.81736 -3.56543 3.16303  
 C 3.03857 -4.05708 2.59600  
 C 3.00407 -4.65624 1.29734  
 C 4.20564 -4.89632 0.60163  
 C 4.18873 -4.87024 -0.84766  
 C 2.97131 -4.60826 -1.50666  
 C 2.97591 -3.96561 -2.78499  
 C 1.74235 -3.45490 -3.30627  
 C 1.76646 -2.34050 -4.15960  
 C 0.54837 -1.65835 -4.45645  
 C 3.12875 -1.89026 4.37249  
 C 4.32106 -2.58739 4.09314  
 C 4.27434 -3.70713 3.17427  
 C 5.44896 -4.26346 2.59233  
 C 5.41608 -4.83874 1.34996  
 C 4.19773 -3.59590 -3.38055  
 C 5.38594 -4.16870 -2.84412  
 C 5.38161 -4.78452 -1.62085  
 C 4.22299 -2.44658 -4.26315  
 C 3.02519 -1.74089 -4.49200  
 C 0.59009 -0.26116 -4.74629  
 C 1.84814 0.41205 -4.73296  
 C 3.06707 -0.34057 -4.78387  
 C 4.30605 0.32762 -4.84159  
 C 5.47848 -0.47561 -4.93143  
 C 5.43837 -1.81587 -4.65300  
 C -1.86360 -0.18896 -4.69626  
 C -0.60556 0.48433 -4.71804  
 C -0.55593 1.87071 -4.38215  
 C 0.68717 2.46246 -4.08235  
 C 1.89699 1.77513 -4.40002  
 C 3.16424 2.38282 -4.11738  
 C 4.35657 1.73503 -4.49769  
 C 0.73387 3.56756 -3.18014  
 C 1.98916 3.95267 -2.62160  
 C 3.21097 3.48993 -3.21192  
 C 4.44944 3.92856 -2.70285  
 C 5.62607 3.46773 -3.35900  
 C 5.58135 2.40865 -4.22651  
 C -3.08378 0.56440 -4.69150  
 C -3.03306 1.95451 -4.35568  
 C -1.76593 2.54209 -4.03375

C -1.72021 3.62816 -3.14570  
 C -0.46420 4.04146 -2.60886  
 C -0.42948 4.64679 -1.31665  
 C 0.80248 4.75495 -0.64084  
 C 2.02340 4.54734 -1.35029  
 C 3.28007 4.67703 -0.67229  
 C 4.48506 4.54273 -1.39027  
 C 0.81900 4.73053 0.78663  
 C 2.05585 4.50000 1.46051  
 C 3.29661 4.65271 0.75869  
 C 4.51774 4.49478 1.44379  
 C 5.71499 4.70065 0.70073  
 C 5.69921 4.72415 -0.66861  
 C -2.94173 4.12448 -2.58261  
 C -2.90695 4.73002 -1.28651  
 C -1.65163 4.81811 -0.59958  
 C -1.63551 4.79369 0.80394  
 C -0.39717 4.59861 1.48633  
 C -0.40257 3.95035 2.75802  
 C 0.80822 3.45766 3.28503  
 C 2.05048 3.86289 2.71162  
 C 3.28538 3.38135 3.25815  
 C 4.51203 3.83791 2.73614  
 C 0.78213 2.32176 4.14906  
 C 1.99892 1.62579 4.41663  
 C 3.25935 2.24395 4.12641  
 C 4.46010 1.58537 4.45830  
 C 5.67824 2.26899 4.18250  
 C 5.70339 3.35648 3.35006  
 C -2.87496 4.68100 1.51599  
 C -2.87995 4.03194 2.79132  
 C -1.64588 3.51792 3.30912  
 C -1.67114 2.40114 4.15953  
 C -0.45366 1.71893 4.45665  
 C -0.49588 0.32265 4.75017  
 C 0.70024 -0.42186 4.72806  
 C 1.95763 0.25270 4.70644  
 C 3.17767 -0.49970 4.70661  
 C 4.41765 0.16740 4.75733  
 C 5.54514 -1.96830 4.47452  
 C 5.59180 -0.63765 4.79464  
 C -2.93016 1.80223 4.49194  
 C -2.97268 0.40237 4.78583  
 C -1.75363 -0.35101 4.73871  
 C -4.21209 -0.26472 4.84823  
 C -5.38440 0.53860 4.93657  
 C -5.34333 1.87827 4.65528  
 C -4.12800 2.50841 4.26453  
 C -4.10224 3.66052 3.38545  
 C -5.29040 4.23540 2.85119  
 C -5.28580 4.85519 1.62986  
 C -4.09262 4.94369 0.85751  
 C -4.10913 4.97016 -0.59185  
 C -5.31944 4.91112 -1.34043  
 C -5.35252 4.33340 -2.58161  
 C -4.17779 3.77459 -3.16083  
 C -4.22506 2.65212 -4.07633  
 C -5.44963 2.03418 -4.45796  
 C -5.49881 0.70390 -4.77911  
 C -4.32497 -0.10100 -4.74347  
 N -2.60865 -1.23725 -0.69825  
 C -1.12221 -1.00600 -0.61973  
 C -0.69449 -0.84928 0.82611  
 H 6.59240 3.88359 -3.09679  
 H 6.51353 2.02212 -4.62228  
 H 6.44092 -0.01251 -5.11670  
 H 6.36969 -2.36978 -4.62790  
 H 6.33388 -4.02874 -3.35091  
 H 6.32584 -5.11203 -1.20124  
 H 6.34981 -5.15451 0.89875  
 H 6.40837 -4.14236 3.08216  
 H 6.47618 -2.51977 4.41092  
 H 6.55839 -0.18031 4.97253  
 H 6.61907 1.87136 4.54545  
 H 6.66320 3.78256 3.08111

H 6.67172 4.73339 1.20946  
 H 6.64395 4.77474 -1.19782  
 H -6.52652 -1.80443 -4.52864  
 H -6.57059 -3.71806 -3.06862  
 H -6.57568 -4.67452 -1.19750  
 H -6.54664 -4.71347 1.20922  
 H -6.49909 -3.81982 3.10686  
 H -6.41970 -1.95773 4.63181  
 H -6.34698 0.07658 5.12372  
 H -6.27445 2.43268 4.63012  
 H -6.23844 4.09373 3.35736  
 H -6.23003 5.18356 1.21073  
 H -6.25317 5.22818 -0.88991  
 H -6.31174 4.21228 -3.07173  
 H -6.37996 2.58674 -4.39418  
 H -6.46588 0.24779 -4.95733  
 H -1.15349 0.02844 1.28999  
 H 0.39034 -0.73356 0.86721  
 H -0.96131 -1.73651 1.40725  
 H -0.64965 -1.86953 -1.09309  
 H -0.91709 -0.11681 -1.21753  
 H -2.93030 -1.34411 -1.66770  
 H -2.88643 -2.08447 -0.18717  
 H -3.12721 -0.45309 -0.28945

# Ethylammonium-graphene, CPCM

C 3.71500 5.66081 -0.14624  
 C 2.96765 4.47388 -0.14195  
 C 3.65572 3.23486 -0.13723  
 C 5.08028 3.22225 -0.12691  
 C 5.80576 4.44444 -0.12636  
 C 5.09913 5.64806 -0.13859  
 C 5.78212 1.98866 -0.11670  
 C 7.22244 1.98482 -0.10198  
 C 7.92276 3.24730 -0.10177  
 C 7.24696 4.41696 -0.11414  
 C 2.93596 2.00019 -0.14421  
 C 3.63660 0.77809 -0.13738  
 C 5.06879 0.77226 -0.12040  
 C 5.77420 -0.45965 -0.10872  
 C 7.21098 -0.45313 -0.09004  
 C 7.89959 0.78746 -0.08841  
 C 2.92886 -0.46207 -0.14614  
 C 3.63471 -1.68125 -0.13566  
 C 5.07239 -1.68389 -0.11454  
 C 5.78999 -2.90700 -0.09964  
 C 7.22160 -2.88933 -0.07629  
 C 7.89975 -1.66275 -0.07373  
 C 5.10222 -4.15633 -0.10557  
 C 3.63735 -4.15217 -0.13753  
 C 2.92724 -2.92031 -0.14719  
 C 1.49960 -2.91652 -0.17347  
 C 0.78662 -1.67774 -0.18618  
 C 1.49584 -0.45787 -0.17096  
 C 0.79310 0.78537 -0.17860  
 C 1.50292 2.00546 -0.16104  
 C 0.79682 3.24707 -0.15658  
 C 1.51001 4.47625 -0.14155  
 C 5.84744 -5.32836 -0.08086  
 C 7.25422 -5.30829 -0.05655  
 C 7.93376 -4.11700 -0.05582  
 C 0.79092 -4.14496 -0.19096  
 C 1.52121 -5.33511 -0.18964  
 C 2.90375 -5.33794 -0.16340  
 C -0.63970 0.78980 -0.20090  
 C -1.35077 -0.45049 -0.22068  
 C -0.64793 -1.67461 -0.21825  
 C -1.36903 -2.90917 -0.23118  
 C -0.66687 -4.14158 -0.21305  
 C -0.63154 3.25202 -0.16159  
 C -1.34425 2.01431 -0.18528  
 C -2.78602 -0.44762 -0.22367  
 C -3.49964 -1.66323 -0.23946  
 C -2.79775 -2.90542 -0.24855

|                        |          |          |          |   |          |          |          |   |          |          |          |
|------------------------|----------|----------|----------|---|----------|----------|----------|---|----------|----------|----------|
| C                      | -3.51474 | -4.13320 | -0.25651 | C | 4.54104  | 1.49812  | 2.29390  | C | -1.00965 | -1.74547 | -4.25769 |
| C                      | -2.78677 | -5.32228 | -0.23307 | C | 5.08164  | 0.31800  | 2.90329  | C | -2.26872 | -1.22672 | -3.89610 |
| C                      | -1.40408 | -5.32751 | -0.21062 | C | 6.21150  | -0.30903 | 2.34249  | C | -2.61691 | 0.11115  | -4.25236 |
| C                      | -3.48833 | 0.79813  | -0.20156 | C | 4.30722  | -0.36314 | 3.89547  | C | -3.90363 | 0.63758  | -3.90276 |
| C                      | -2.77924 | 2.01713  | -0.18409 | C | 4.67647  | -1.65971 | 4.30716  | C | -4.27215 | 1.93381  | -4.31567 |
| C                      | -4.92157 | 0.79970  | -0.20118 | C | 5.98300  | -2.10807 | 3.96213  | C | -3.03945 | -1.90162 | -2.90240 |
| C                      | -5.63300 | -0.42896 | -0.22339 | C | 6.72460  | -1.45520 | 3.01366  | C | -4.13506 | -1.21759 | -2.29661 |
| C                      | -4.93771 | -1.65733 | -0.24190 | C | 3.02005  | 0.16138  | 4.24627  | C | -4.67657 | -0.03856 | -2.90641 |
| C                      | -5.66157 | -2.87650 | -0.26491 | C | 2.67121  | 1.49959  | 3.89176  | C | -5.80509 | 0.59091  | -2.34475 |
| C                      | -4.97995 | -4.12986 | -0.28093 | C | 3.44276  | 2.17757  | 2.90023  | C | -6.31873 | 1.73557  | -3.01740 |
| C                      | -1.33846 | 4.48430  | -0.14371 | C | 2.92767  | 3.34814  | 2.30745  | C | -5.57763 | 2.38431  | -3.96911 |
| C                      | -0.60132 | 5.67109  | -0.12334 | C | 3.30072  | 3.67504  | 0.96879  | C | 1.64580  | -2.71547 | -4.70181 |
| C                      | 0.77948  | 5.66729  | -0.12310 | C | 4.17686  | 2.82067  | 0.27020  | C | 0.62268  | -3.61089 | -4.25477 |
| C                      | -2.79657 | 4.49051  | -0.14468 | C | 4.07831  | 2.73127  | -1.15136 | C | -0.64819 | -3.07099 | -3.86999 |
| C                      | -3.49269 | 3.25603  | -0.16226 | C | 4.71551  | 1.64449  | -1.82263 | C | -1.40839 | -3.73632 | -2.89477 |
| C                      | -4.91723 | 3.24988  | -0.16239 | C | 2.01753  | -0.71739 | 4.68723  | C | -2.52689 | -3.07307 | -2.30849 |
| C                      | -5.62656 | 2.02004  | -0.18206 | C | 2.30532  | -2.11907 | 4.77624  | C | -2.89784 | -3.39759 | -0.96854 |
| C                      | -7.06691 | 2.02368  | -0.18360 | C | 3.64140  | -2.56674 | 4.76283  | C | -3.76654 | -2.53505 | -0.26894 |
| C                      | -7.75073 | 0.83034  | -0.20601 | C | 1.41300  | 2.01757  | 4.25747  | C | -4.49697 | -1.53256 | -0.97725 |
| C                      | -7.07006 | -0.41464 | -0.22754 | C | 0.39373  | 1.12406  | 4.70601  | C | -5.40535 | -0.67335 | -0.27459 |
| C                      | -7.76503 | -1.62068 | -0.25432 | C | 0.66965  | -0.25640 | 4.77370  | C | -6.18470 | 0.26107  | -0.98573 |
| C                      | -7.09349 | -2.85052 | -0.27496 | C | -0.39474 | -1.18963 | 4.58841  | C | -3.67302 | -2.45044 | 1.15462  |
| C                      | -7.81144 | -4.07499 | -0.30672 | C | -0.07901 | -2.55640 | 4.32436  | C | -4.30829 | -1.36147 | 1.82675  |
| C                      | -7.13771 | -5.26912 | -0.32991 | C | 1.23812  | -3.05470 | 4.59234  | C | -5.30811 | -0.58531 | 1.15233  |
| C                      | -5.73071 | -5.29767 | -0.31775 | C | 1.52675  | -4.42050 | 4.40053  | C | -5.98949 | 0.43906  | 1.84022  |
| C                      | -5.63545 | 4.47594  | -0.14362 | C | 2.84087  | -4.86247 | 4.72411  | C | -7.00565 | 1.13831  | 1.12892  |
| C                      | -7.07691 | 4.45609  | -0.14322 | C | 3.86241  | -3.96705 | 4.89871  | C | -7.10083 | 1.05161  | -0.23467 |
| C                      | -7.75944 | 3.29052  | -0.16224 | C | 1.05024  | 3.34321  | 3.87176  | C | -0.89657 | -4.93959 | -2.30638 |
| C                      | -4.92157 | 5.67513  | -0.12708 | C | 1.80805  | 4.00884  | 2.89513  | C | -1.27097 | -5.26644 | -0.96398 |
| C                      | -3.53731 | 5.68128  | -0.12808 | C | -1.69693 | -0.70970 | 4.34356  | C | -2.14383 | -3.37739 | -0.25519 |
| C                      | -0.71744 | -0.45010 | 3.10455  | C | -2.00380 | 0.66517  | 4.57400  | C | -2.04797 | -4.29101 | 1.14408  |
| N                      | -1.64512 | 0.73103  | 3.00712  | C | -0.95688 | 1.58287  | 4.75623  | C | -2.70722 | -3.22562 | 1.82847  |
| C                      | -1.51368 | -1.73942 | 3.10255  | C | -1.24148 | 2.98737  | 4.70978  | C | -2.15814 | -2.73874 | 3.05312  |
| H                      | -7.60095 | 5.40719  | -0.12737 | C | -0.21939 | 3.88290  | 4.26050  | C | -2.59343 | -1.49693 | 3.56009  |
| H                      | 7.77626  | 5.36524  | -0.11445 | C | -0.54602 | 5.21607  | 3.94076  | C | -3.76960 | -0.88551 | 3.03282  |
| H                      | -8.85169 | -1.60974 | -0.26022 | C | 0.23527  | 5.90235  | 2.93113  | C | -4.23018 | 0.36635  | 3.55769  |
| H                      | -8.83753 | 0.83112  | -0.20815 | C | 1.29348  | 5.21161  | 2.30796  | C | -5.43064 | 0.93196  | 3.08252  |
| H                      | -8.84518 | 3.27887  | -0.16223 | C | 1.66554  | 5.53776  | 0.96481  | C | -4.99530 | 2.91051  | 4.42526  |
| H                      | -8.89665 | -4.04436 | -0.31457 | C | 2.54142  | 4.65136  | 0.25632  | C | -5.85588 | 2.15575  | 3.67325  |
| H                      | -7.68490 | -6.20536 | -0.35813 | C | 2.44509  | 4.56399  | -1.14161 | C | -1.07779 | -5.09216 | 1.83061  |
| H                      | -5.24477 | -6.26515 | -0.34129 | C | 3.10814  | 3.49996  | -1.82430 | C | -0.52598 | -4.60350 | 3.05759  |
| H                      | -3.29579 | -6.27783 | -0.22499 | C | -3.33147 | 1.15470  | 4.34433  | C | -0.96229 | -3.33183 | 3.55597  |
| H                      | -0.90513 | -6.28743 | -0.18609 | C | -3.65008 | 2.49552  | 4.63920  | C | 0.61469  | -5.22051 | 3.60745  |
| H                      | 1.01673  | -6.29222 | -0.21299 | C | -2.56960 | 3.44223  | 4.83143  | C | 0.97152  | -6.50274 | 3.10159  |
| H                      | 3.40737  | -6.29633 | -0.16662 | C | -2.78192 | 4.85021  | 4.82237  | C | 0.44363  | -6.97032 | 1.92726  |
| H                      | 5.35634  | -6.29355 | -0.07824 | C | -1.80404 | 5.70720  | 4.39251  | C | -0.47965 | -6.18798 | 1.17670  |
| H                      | 7.79621  | -6.24769 | -0.03833 | C | 0.97133  | 6.54777  | 0.26856  | C | -0.57971 | -6.27807 | -0.26712 |
| H                      | 9.01901  | -4.09163 | -0.03813 | C | 0.15101  | 7.42346  | 1.03575  | C | 0.23939  | -7.15502 | -1.03395 |
| H                      | 8.98641  | -1.65758 | -0.05806 | C | -0.20376 | 7.11226  | 2.32156  | C | 0.59739  | -6.84240 | -2.31856 |
| H                      | 8.98633  | 0.78178  | -0.07612 | C | 0.87234  | 6.45780  | -1.17515 | C | 0.16246  | -5.63077 | -2.92754 |
| H                      | 9.00837  | 3.22920  | -0.09172 | C | 1.47355  | 5.36311  | -1.82834 | C | 0.94768  | -4.94429 | -3.93419 |
| H                      | -5.46513 | 6.61509  | -0.11363 | C | 2.55833  | 3.01151  | -3.04810 | C | 2.20757  | -5.43523 | -4.38050 |
| H                      | -3.03414 | 6.63958  | -0.11567 | C | 1.36290  | 3.60352  | -3.55394 | C | 3.18674  | -4.57780 | -4.80694 |
| H                      | -1.10297 | 6.62996  | -0.10603 | C | 0.92438  | 4.87497  | -3.05678 | C | 2.97445  | -3.16986 | -4.81856 |
| H                      | 1.28633  | 6.62335  | -0.10389 | C | -0.21472 | 5.49210  | -3.60976 | C | 4.05472  | -2.22236 | -4.62720 |
| H                      | 3.21680  | 6.62180  | -0.15803 | C | -0.57481 | 6.77327  | -3.10337 | C | 5.40008  | -2.63608 | -4.41275 |
| H                      | 5.64776  | 6.58509  | -0.14182 | C | -0.05067 | 7.23951  | -1.92689 | C | 6.26015  | -1.87791 | -3.66344 |
| H                      | -2.10974 | -1.83687 | 4.01261  | C | 4.17294  | 1.16264  | -3.02502 | C | 5.83520  | -0.65248 | -3.07540 |
| H                      | -2.18048 | -1.79349 | 2.23693  | C | 2.99609  | 1.77094  | -3.55454 | C | -6.54843 | -4.45716 | -0.62736 |
| H                      | -0.82241 | -2.58285 | 3.04929  | C | 2.10008  | 0.98189  | -4.33738 | N | -7.10406 | -3.44755 | 0.34109  |
| H                      | -0.14718 | -0.31737 | 4.02335  | C | 0.79880  | 1.46138  | -4.58755 | C | -5.70203 | -5.47532 | 0.10876  |
| H                      | -0.03795 | -0.37765 | 2.25365  | C | 0.48210  | 2.82818  | -4.32501 | H | -4.46244 | 4.62044  | -5.05465 |
| H                      | -1.13557 | 1.61885  | 3.03472  | C | -0.83399 | 3.32652  | -4.59751 | H | -2.66737 | 6.19340  | -4.74298 |
| H                      | -2.18911 | 0.70710  | 2.13608  | C | -1.12362 | 4.69218  | -4.40637 | H | -1.35253 | 7.35009  | -3.59053 |
| H                      | -2.31613 | 0.74074  | 3.78162  | C | -0.26512 | 0.52792  | -4.77425 | H | -0.43071 | 8.17063  | -1.52224 |
| Ethylammonium-convex   |          |          |          | C | -1.61344 | 0.98920  | -4.69226 | H | -0.29003 | 8.29891  | 0.57291  |
| surface of SWCNT, CPCM |          |          |          | C | -1.90098 | 2.39100  | -4.78334 | H | -0.91339 | 7.75171  | 2.83391  |
| C                      | 7.50825  | -0.76822 | 0.23638  | C | -3.23698 | 2.83919  | -4.77392 | H | -2.04082 | 6.76096  | 4.29881  |
| C                      | 6.59349  | 0.02569  | 0.98515  | C | -3.45777 | 4.23923  | -4.91267 | H | -3.76059 | 5.25408  | 5.05527  |
| C                      | 5.81850  | 0.96383  | 0.27503  | C | -2.43648 | 5.13423  | -4.73536 | H | -5.32324 | 3.88568  | 4.76666  |
| C                      | 5.71932  | 0.87383  | -1.14961 | C | 4.63400  | -0.08946 | -3.55012 | H | -6.83578 | 2.55862  | 3.44453  |
| C                      | 6.39684  | -0.15369 | -1.83613 | C | 3.73530  | -0.88133 | -4.33358 | H | -7.65232 | 1.83453  | 1.65081  |
| C                      | 7.41306  | -0.85518 | -1.12681 | C | 2.40753  | -0.39315 | -4.56605 | H | -7.82006 | 1.68144  | -0.74558 |
| C                      | 4.90955  | 1.82092  | 0.97802  | C | 1.36124  | -1.31116 | -4.75044 | H | -7.25975 | 2.17298  | -2.70412 |
|                        |          |          |          | C | 0.01056  | -0.85254 | -4.70533 | H | -5.95846 | 3.31336  | -4.37773 |

|   |          |          |          |
|---|----------|----------|----------|
| H | 8.05724  | -1.55366 | -1.64893 |
| H | 8.22509  | -1.40022 | 0.74816  |
| H | 7.66729  | -1.89010 | 2.70170  |
| H | 6.36467  | -3.03732 | 4.36963  |
| H | 4.86766  | -4.34829 | 5.03645  |
| H | 3.07237  | -5.92151 | 4.72962  |
| H | 1.74982  | -7.07992 | 3.58739  |
| H | 0.82157  | -7.90240 | 1.52301  |
| H | 0.67767  | -8.03206 | -0.57162 |
| H | 1.30656  | -7.48279 | -2.83036 |
| H | 2.44478  | -6.48869 | -4.28478 |
| H | 4.16657  | -4.98162 | -5.03510 |
| H | 5.72893  | -3.61171 | -4.75205 |
| H | 7.24086  | -2.27914 | -3.43502 |
| H | -6.29997 | -6.04826 | 0.82108  |
| H | -5.27407 | -6.16862 | -0.61709 |
| H | -4.87794 | -4.97512 | 0.64474  |
| H | -7.40608 | -4.91124 | -1.12260 |
| H | -5.97221 | -3.89279 | -1.36141 |
| H | -7.65232 | -2.72389 | -0.13339 |
| H | -6.35404 | -2.97820 | 0.86136  |
| H | -7.71713 | -3.89314 | 1.03052  |

# Propanoate-concave surface of SWCNT, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.56301  | -4.66414 | 1.38131  |
| C | 4.36157  | -4.76562 | 0.62279  |
| C | 3.14581  | -4.57812 | 1.30992  |
| C | 3.14771  | -3.98257 | 2.61143  |
| C | 4.36455  | -3.58904 | 3.20296  |
| C | 5.56471  | -4.09549 | 2.62732  |
| C | 1.90062  | -4.71071 | 0.61162  |
| C | 1.89312  | -4.67615 | -0.79172 |
| C | 3.13226  | -4.50924 | -1.49262 |
| C | 4.35448  | -4.72940 | -0.82647 |
| C | 3.12027  | -3.84944 | -2.76274 |
| C | 4.33257  | -3.42066 | -3.34021 |
| C | 5.53888  | -3.95377 | -2.80213 |
| C | 5.54983  | -4.58664 | -1.58756 |
| C | 1.87180  | -3.38144 | -3.28511 |
| C | 0.64434  | -3.86733 | -2.74700 |
| C | 0.65441  | -4.52735 | -1.48324 |
| C | -0.55976 | -4.71632 | -0.79383 |
| C | -0.55331 | -4.74440 | 0.63389  |
| C | 0.66779  | -4.59133 | 1.32049  |
| C | 0.66918  | -3.99822 | 2.61863  |
| C | 1.90354  | -3.54141 | 3.17074  |
| C | 1.85962  | -2.25080 | -4.11561 |
| C | 3.09490  | -1.59606 | -4.42821 |
| C | 4.31951  | -2.25702 | -4.20350 |
| C | -0.58019 | -3.41845 | -3.27691 |
| C | -0.59274 | -2.26376 | -4.11533 |
| C | 0.61979  | -1.60687 | -4.39956 |
| C | 0.60739  | -0.20782 | -4.67192 |
| C | 1.83607  | 0.51380  | -4.65401 |
| C | 3.08313  | -0.19053 | -4.70268 |
| C | 4.29635  | 0.52574  | -4.75006 |
| C | 5.50040  | -0.22938 | -4.84118 |
| C | 5.51158  | -1.57331 | -4.57718 |
| C | -1.80995 | -3.88053 | -2.71913 |
| C | -1.80041 | -4.52965 | -1.47392 |
| C | -0.61534 | 0.48999  | -4.65492 |
| C | -1.84406 | -0.23306 | -4.65266 |
| C | -1.83268 | -1.61092 | -4.38113 |
| C | -3.07066 | -2.28137 | -4.11180 |
| C | -3.05941 | -3.43460 | -3.26386 |
| C | -4.27218 | -3.94385 | -2.75703 |
| C | -4.26160 | -4.61538 | -1.47283 |
| C | -3.03928 | -4.73310 | -0.78147 |
| C | -3.03251 | -4.76788 | 0.64960  |
| C | -1.78645 | -4.59226 | 1.33692  |
| C | -1.78519 | -4.01047 | 2.61456  |
| C | -0.55066 | -3.58160 | 3.18771  |
| C | -3.09310 | 0.47037  | -4.66384 |
| C | -4.30550 | -0.24511 | -4.73132 |

|   |          |          |          |
|---|----------|----------|----------|
| C | -4.29388 | -1.66603 | -4.44535 |
| C | -5.48680 | -2.39993 | -4.18901 |
| C | -5.47690 | -3.49925 | -3.37222 |
| C | -4.24687 | -4.69061 | 1.36077  |
| C | -5.44802 | -4.91270 | 0.62881  |
| C | -5.45494 | -4.87486 | -0.74026 |
| C | -4.24507 | -4.09097 | 2.68031  |
| C | -3.02892 | -3.60758 | 3.20293  |
| C | -0.55525 | -2.48857 | 4.10569  |
| C | -1.79456 | -1.85596 | 4.42299  |
| C | -3.03383 | -2.51155 | 4.12303  |
| C | -4.25433 | -1.91861 | 4.50300  |
| C | -5.44842 | -2.63916 | 4.21539  |
| C | -5.44389 | -3.68826 | 3.33485  |
| C | 1.89909  | -2.46695 | 4.07426  |
| C | 0.66028  | -1.85032 | 4.42336  |
| C | 0.65006  | -0.46759 | 4.77861  |
| C | -0.57524 | 0.22788  | 4.80413  |
| C | -1.80471 | -0.49611 | 4.77182  |
| C | -3.05408 | 0.20540  | 4.81902  |
| C | -4.26508 | -0.51390 | 4.86076  |
| C | -0.58864 | 1.62823  | 4.52635  |
| C | -1.83076 | 2.26230  | 4.22348  |
| C | -3.06736 | 1.60908  | 4.53904  |
| C | -4.29118 | 2.26703  | 4.30483  |
| C | -5.48289 | 1.58269  | 4.67788  |
| C | -5.47036 | 0.23964  | 4.94631  |
| C | 3.13891  | -1.83214 | 4.41372  |
| C | 3.12883  | -0.44580 | 4.77022  |
| C | 1.87942  | 0.25736  | 4.77507  |
| C | 1.86615  | 1.63481  | 4.50296  |
| C | 0.62395  | 2.28398  | 4.23369  |
| C | 0.61081  | 3.42539  | 3.37628  |
| C | -0.61445 | 3.87033  | 2.84078  |
| C | -1.84369 | 3.38364  | 3.37850  |
| C | -3.09309 | 3.85022  | 2.85245  |
| C | -4.30454 | 3.42532  | 3.43345  |
| C | -0.62461 | 4.52722  | 1.57336  |
| C | -1.86357 | 4.67819  | 0.88146  |
| C | -3.10310 | 4.50886  | 1.58192  |
| C | -4.32477 | 4.73026  | 0.91568  |
| C | -5.51979 | 4.58618  | 1.67658  |
| C | -5.51029 | 3.95597  | 2.89273  |
| C | 3.10259  | 2.30637  | 4.22785  |
| C | 3.08922  | 3.45182  | 3.36963  |
| C | 1.84007  | 3.88543  | 2.81551  |
| C | 1.83001  | 4.53064  | 1.56832  |
| C | 0.59048  | 4.71492  | 0.88474  |
| C | 0.58491  | 4.75748  | -0.54238 |
| C | -0.63522 | 4.60892  | -1.23228 |
| C | -1.86871 | 4.71979  | -0.52221 |
| C | -3.11411 | 4.59262  | -1.22124 |
| C | -4.33039 | 4.77598  | -0.53325 |
| C | -0.63482 | 4.03072  | -2.53742 |
| C | -1.86869 | 3.57769  | -3.09268 |
| C | -3.11347 | 4.01021  | -2.52844 |
| C | -4.33074 | 3.61713  | -3.11963 |
| C | -5.53144 | 4.11916  | -2.54146 |
| C | -5.53166 | 4.68073  | -1.29231 |
| C | 3.06929  | 4.74205  | 0.87905  |
| C | 3.06341  | 4.78255  | -0.55201 |
| C | 1.81913  | 4.61059  | -1.24352 |
| C | 1.81835  | 4.03389  | -2.52337 |
| C | 0.58532  | 3.61108  | -3.10287 |
| C | 0.59038  | 2.51558  | -4.01422 |
| C | -0.62421 | 1.87721  | -4.32652 |
| C | -1.86268 | 2.50140  | -3.99471 |
| C | -3.10270 | 1.86188  | -4.32708 |
| C | -4.32514 | 2.50602  | -4.04998 |
| C | -5.51109 | 0.51154  | -4.77429 |
| C | -5.52085 | 1.84040  | -4.44393 |
| C | 3.06366  | 3.62767  | -3.10628 |
| C | 3.06734  | 2.52912  | -4.02323 |
| C | 1.82698  | 1.87644  | -4.32035 |
| C | 4.28810  | 1.93092  | -4.39566 |

|   |          |          |          |
|---|----------|----------|----------|
| C | 5.48352  | 2.64907  | -4.10650 |
| C | 5.47998  | 3.70119  | -3.22959 |
| C | 4.27966  | 4.10870  | -2.58058 |
| C | 4.27933  | 4.70662  | -1.26031 |
| C | 5.47870  | 4.92882  | -0.52516 |
| C | 5.48422  | 4.89175  | 0.84394  |
| C | 4.29004  | 4.62957  | 1.57422  |
| C | 4.30035  | 3.96218  | 2.86093  |
| C | 5.50544  | 3.52431  | 3.48082  |
| C | 5.51796  | 2.42858  | 4.30223  |
| C | 4.32643  | 1.69294  | 4.56115  |
| C | 4.34044  | 0.27033  | 4.83994  |
| C | 5.54632  | -0.48655 | 4.87091  |
| C | 5.55567  | -1.81280 | 4.52965  |
| C | 4.36005  | -2.47676 | 4.13267  |
| O | 0.56355  | 0.83612  | -1.56174 |
| C | 0.31649  | -0.34226 | -1.20631 |
| O | 1.13449  | -1.29109 | -1.09559 |
| C | -1.15225 | -0.68584 | -0.84397 |
| C | -2.11629 | 0.48965  | -0.89495 |
| H | -6.43635 | 2.09777  | 4.64749  |
| H | -6.41483 | -0.26329 | 5.12000  |
| H | -6.39804 | -2.29544 | 4.60944  |
| H | -6.39037 | -4.14085 | 3.06160  |
| H | -6.39379 | -5.00626 | 1.15031  |
| H | -6.40625 | -4.93917 | -1.25629 |
| H | -6.42184 | -3.96478 | -3.11580 |
| H | -6.43928 | -2.03211 | -4.55337 |
| H | -6.45694 | 0.01699  | -4.96448 |
| H | -6.47392 | 2.35341  | -4.38141 |
| H | -6.48110 | 3.96551  | -3.04133 |
| H | -6.48064 | 4.95383  | -0.84473 |
| H | -6.47288 | 4.87942  | 1.25128  |
| H | -6.45596 | 3.77116  | 3.38952  |
| H | 6.51479  | -3.94045 | 3.12584  |
| H | 6.51177  | -4.93996 | 0.93483  |
| H | 6.50302  | -4.88107 | -1.16317 |
| H | 6.48422  | -3.76745 | -3.29927 |
| H | 6.46415  | -2.09062 | -4.55274 |
| H | 6.44493  | 0.27260  | -5.01811 |
| H | 6.43358  | 2.30040  | -4.49541 |
| H | 6.42704  | 4.15105  | -2.95371 |
| H | 6.42521  | 5.02396  | -1.04513 |
| H | 6.43458  | 4.95871  | 1.36126  |
| H | 6.44932  | 3.99161  | 3.22393  |
| H | 6.47107  | 2.06425  | 4.66829  |
| H | 6.49265  | 0.00690  | 5.06117  |
| H | 6.50899  | -2.32444 | 4.46140  |
| H | -1.80047 | 1.28711  | -0.21335 |
| H | -2.12775 | 0.91818  | -1.90051 |
| H | -3.13752 | 0.19409  | -0.63029 |
| H | -1.14448 | -1.15041 | 0.15238  |
| H | -1.48076 | -1.47855 | -1.52900 |

# Propanoate-graphene, CPCM

|   |          |          |          |
|---|----------|----------|----------|
| C | -3.54321 | 5.61827  | -0.34227 |
| C | -2.79848 | 4.42983  | -0.31243 |
| C | -3.48817 | 3.19111  | -0.31681 |
| C | -4.91300 | 3.18217  | -0.34457 |
| C | -5.63574 | 4.40584  | -0.37216 |
| C | -4.92715 | 5.60823  | -0.37173 |
| C | -2.76992 | 1.95621  | -0.29447 |
| C | -1.33839 | 1.95913  | -0.26532 |
| C | -0.63151 | 3.19829  | -0.25803 |
| C | -1.34155 | 4.42899  | -0.27526 |
| C | -0.62991 | 0.74002  | -0.25303 |
| C | 0.80085  | 0.74205  | -0.22188 |
| C | 1.50674  | 1.96377  | -0.21753 |
| C | 0.79606  | 3.20140  | -0.22373 |
| C | 2.93994  | 1.96486  | -0.19390 |
| C | 3.64774  | 0.74646  | -0.19533 |
| C | 2.94436  | -0.49624 | -0.20252 |
| C | 1.51093  | -0.49658 | -0.22316 |
| C | 1.50342  | 4.43350  | -0.21015 |



C 2.96099 4.43882 -0.18144  
 C 3.65534 3.20265 -0.18002  
 C 5.08020 3.19662 -0.16030  
 C 5.79926 4.42246 -0.14089  
 C 5.08676 5.62252 -0.13902  
 C 3.70264 5.62935 -0.15890  
 C 5.08034 0.74698 -0.17778  
 C 5.78823 1.96640 -0.16231  
 C 7.22867 1.96791 -0.14682  
 C 7.92209 3.23440 -0.12659  
 C 7.24049 4.40088 -0.12314  
 C 5.79203 -0.48230 -0.18059  
 C 7.22968 -0.47035 -0.16954  
 C 7.91193 0.77401 -0.15190  
 C 3.65604 -1.71204 -0.20270  
 C 5.09429 -1.70947 -0.19208  
 C 5.81726 -2.93021 -0.19600  
 C 7.24947 -2.90657 -0.19127  
 C 7.92300 -1.67750 -0.17661  
 C 0.80633 -1.71905 -0.21623  
 C 1.52517 -2.95481 -0.20475  
 C 2.95351 -2.95358 -0.20306  
 C 3.66820 -4.18285 -0.20217  
 C 5.13379 -4.18274 -0.20605  
 C 5.88277 -5.35262 -0.21793  
 C 7.28967 -5.32617 -0.21586  
 C 7.96518 -4.13271 -0.20132  
 C 0.82143 -4.18665 -0.19157  
 C 1.55598 -5.37443 -0.19142  
 C 2.93878 -5.37149 -0.19683  
 C -0.63636 -4.18776 -0.18420  
 C -1.34273 -2.95793 -0.21323  
 C -0.62818 -1.72010 -0.23294  
 C -1.33481 -0.49957 -0.24124  
 C -0.61089 5.62052 -0.25537  
 C 0.76912 5.62278 -0.22402  
 C -3.47348 0.73699 -0.28930  
 C -2.76742 -0.50229 -0.26631  
 C -3.47546 -1.71998 -0.25330  
 C -2.77061 -2.96055 -0.22577  
 C -3.48231 -4.19129 -0.20374  
 C -2.75068 -5.37777 -0.15635  
 C -1.36800 -5.37682 -0.14660  
 C -4.90508 0.73330 -0.31459  
 C -5.61428 -0.49740 -0.30598  
 C -4.91380 -1.72213 -0.27508  
 C -5.63369 -2.94458 -0.26462  
 C -4.94755 -4.19490 -0.23076  
 C -5.61737 1.95033 -0.34208  
 C -7.05773 1.94806 -0.36789  
 C -7.73780 0.75238 -0.36214  
 C -7.05159 -0.48947 -0.33033  
 C -7.74207 -1.69814 -0.32229  
 C -7.06558 -2.92532 -0.29003  
 C -7.77865 -4.15287 -0.28278  
 C -7.10056 -5.34463 -0.25375  
 C -5.69380 -5.36662 -0.22868  
 C -7.07679 4.38048 -0.40042  
 C -7.75507 3.21207 -0.39844  
 C -1.08625 0.96916 2.89560  
 O -2.33241 1.00455 2.75197  
 C -0.43077 -0.42237 3.07766  
 C -1.40757 -1.58613 3.15624  
 O -0.29193 1.94374 2.90792  
 H -7.60427 5.32970 -0.42327  
 H 7.76561 5.35156 -0.10706  
 H -8.82873 -1.69194 -0.34100  
 H -8.82453 0.74871 -0.38086  
 H -8.84069 3.19618 -0.41912  
 H -8.86395 -4.12682 -0.30185  
 H -7.64423 -6.28341 -0.25038  
 H -5.20381 -6.33217 -0.20908  
 H -3.25607 -6.33486 -0.12503  
 H -0.86446 -6.33396 -0.10603  
 H 1.05467 -6.33353 -0.19106

H 3.44649 -6.32786 -0.19497  
 H 5.39524 -6.31950 -0.23061  
 H 7.83596 -6.26345 -0.22546  
 H 9.05058 -4.10408 -0.19841  
 H 9.00975 -1.66842 -0.17091  
 H 8.99876 0.77374 -0.14210  
 H 9.00787 3.22194 -0.11396  
 H -5.47400 6.54623 -0.39455  
 H -3.04302 6.57834 -0.34349  
 H -1.11704 6.57723 -0.26388  
 H 1.27231 6.58104 -0.21166  
 H 3.19990 6.58802 -0.15642  
 H 5.63118 6.56209 -0.12188  
 H -2.01582 -1.52772 4.06402  
 H -2.09434 -1.55583 2.30669  
 H -0.89177 -2.55296 3.15351  
 H 0.20008 -0.37827 3.97445  
 H 0.26473 -0.55962 2.23992

# Propanoate-convex surface of SWCNT, CPCM

C -1.00660 -5.43731 -4.84428  
 C 0.04949 -4.53819 -4.52287  
 C -0.20467 -3.16085 -4.67606  
 C -1.55092 -2.69595 -4.81701  
 C -2.61737 -3.61692 -4.80158  
 C -2.29497 -4.99274 -4.97942  
 C 0.83155 -2.20656 -4.40941  
 C 1.96126 -2.60711 -3.67745  
 C 2.05071 -3.96116 -3.21381  
 C 1.21523 -4.95177 -3.76683  
 C 2.77753 -4.23201 -2.01075  
 C 2.65427 -5.48777 -1.38297  
 C 2.07394 -6.54355 -2.14190  
 C 1.37954 -6.28475 -3.29386  
 C 3.39068 -3.13919 -1.31435  
 C 3.58283 -1.88686 -1.97202  
 C 2.85600 -1.61692 -3.17150  
 C 2.77690 -0.29226 -3.64489  
 C 1.62821 0.11525 -4.38853  
 C 0.59975 -0.81649 -4.63422  
 C -0.74308 -0.35240 -4.77540  
 C -1.81362 -1.29226 -4.68646  
 C 3.54740 -3.21629 0.07916  
 C 3.09553 -4.38707 0.77264  
 C 2.81977 -5.56843 0.05522  
 C 4.20396 -0.82289 -1.28921  
 C 4.36311 -0.90163 0.12624  
 C 3.89062 -2.03962 0.80880  
 C 3.46214 -1.91478 2.16406  
 C 2.69436 -2.96631 2.74807  
 C 2.66081 -4.25975 2.13064  
 C 1.96019 -5.31599 2.74671  
 C 1.99826 -6.58667 2.10553  
 C 2.41276 -6.70845 0.80546  
 C 4.36223 0.43927 -1.93359  
 C 3.64735 0.70582 -3.11091  
 C 3.51444 -0.65261 2.78787  
 C 4.25807 0.40676 2.18603  
 C 4.68585 0.28066 0.85498  
 C 5.18455 1.43400 0.16621  
 C 5.01901 1.51504 -1.25205  
 C 5.23649 2.73848 -1.91542  
 C 4.49545 3.01612 -3.13071  
 C 3.58597 2.05048 -3.60558  
 C 2.43450 2.45939 -4.35131  
 C 1.38527 1.50896 -4.57900  
 C 0.06500 1.96512 -4.71998  
 C -1.00979 1.02732 -4.66812  
 C 4.32812 1.68790 2.82666  
 C 5.12038 2.71046 2.26873  
 C 5.56362 2.57854 0.89437  
 C 6.08818 3.67874 0.15789  
 C 5.92929 3.75654 -1.20023  
 C 2.21463 3.82704 -4.61046

C 3.30826 4.71509 -4.40365  
 C 4.40945 4.32323 -3.68940  
 C 0.85121 4.29810 -4.75654  
 C -0.20299 3.37114 -4.63347  
 C -2.28004 1.45621 -4.17700  
 C -2.43773 2.81027 -3.75415  
 C -1.47688 3.80120 -4.14254  
 C -1.67317 5.15018 -3.78603  
 C -0.70511 6.09248 -4.23663  
 C 0.51441 5.68090 -4.70478  
 C -3.06270 -0.87042 -4.20313  
 C -3.23864 0.49048 -3.81064  
 C -4.18296 0.79914 -2.78524  
 C -4.13600 2.06271 -2.16305  
 C -3.36644 3.11387 -2.74596  
 C -3.33260 4.40748 -2.12873  
 C -2.63200 5.46352 -2.74491  
 C -4.56896 2.19029 -0.80857  
 C -4.21892 3.36487 -0.07711  
 C -3.76580 4.53513 -0.77055  
 C -3.48892 5.71614 -0.05315  
 C -3.08292 6.85635 -0.80357  
 C -2.66981 6.73431 -2.10391  
 C -4.04526 -1.85331 -3.85074  
 C -4.99234 -1.54371 -2.82303  
 C -4.92369 -0.26224 -2.18370  
 C -5.35050 -0.13636 -0.85195  
 C -5.03426 1.04979 -0.12400  
 C -4.87092 0.97061 1.29221  
 C -4.24806 2.03513 1.97401  
 C -4.05789 3.28698 1.31568  
 C -3.44418 4.37961 2.01189  
 C -3.32243 5.63560 1.38463  
 C -3.52246 1.76524 3.17366  
 C -2.62738 2.75557 3.67875  
 C -2.71701 4.10908 3.21457  
 C -1.88123 5.09980 3.76700  
 C -2.04657 6.43278 3.29442  
 C -2.74219 6.69163 2.14328  
 C -5.84507 -1.29219 -0.16272  
 C -5.68163 -1.37144 1.25705  
 C -5.02931 -0.29192 1.93835  
 C -4.31547 -0.55734 3.11816  
 C -3.44397 0.44069 3.64875  
 C -2.29578 0.03361 4.39379  
 C -1.26653 0.96510 4.63687  
 C -1.49784 2.35517 4.41091  
 C -0.46123 3.30926 4.67669  
 C -0.71534 4.68656 4.52278  
 C 0.07604 0.50076 4.77909  
 C 1.14691 1.44013 4.68895  
 C 0.88476 2.84393 4.81835  
 C 1.95159 3.76433 4.80142  
 C 1.62938 5.14044 4.97775  
 C 0.34119 5.58565 4.84282  
 C -4.25434 -1.90155 3.61295  
 C -3.10308 -2.30984 4.35965  
 C -2.05348 -1.35979 4.58551  
 C -0.73319 -1.81664 4.72575  
 C 0.34193 -0.87923 4.67231  
 C 1.61194 -1.30893 4.18140  
 C 2.57067 -0.34362 3.81367  
 C 2.39579 1.01764 4.20572  
 C 3.37948 1.99952 3.85250  
 C 3.24108 3.32803 4.30237  
 C 5.17876 3.94767 2.97108  
 C 4.27178 4.24628 3.95304  
 C -0.46611 -3.22296 4.63904  
 C 0.80716 -3.65367 4.14689  
 C 1.76800 -2.66309 3.75828  
 C 1.00181 -5.00246 3.78842  
 C 0.03341 -5.94431 4.23934  
 C -1.18502 -5.53255 4.71017  
 C -1.52056 -4.14951 4.76363  
 C -2.88367 -3.67747 4.61890

|                        |          |          |          |   |          |          |          |   |          |          |          |
|------------------------|----------|----------|----------|---|----------|----------|----------|---|----------|----------|----------|
| C                      | -3.97839 | -4.56499 | 4.41506  | C | -3.07223 | -3.98738 | -2.62304 | C | -0.61531 | -1.66300 | 4.45811  |
| C                      | -5.07993 | -4.17412 | 3.70112  | C | -4.29003 | -3.60284 | -3.21756 | C | 0.60784  | -2.29935 | 4.16663  |
| C                      | -5.16418 | -2.86812 | 3.13973  | C | 0.62171  | -2.42999 | -4.08051 | C | 1.83951  | -1.63633 | 4.44961  |
| C                      | -5.90143 | -2.59402 | 1.92206  | C | 0.62557  | -3.53432 | -3.17397 | C | 3.08640  | -2.28804 | 4.17519  |
| C                      | -6.59152 | -3.61305 | 1.20572  | C | -0.59384 | -3.97450 | -2.61800 | C | 4.29997  | -1.66173 | 4.52192  |
| C                      | -6.74824 | -3.53716 | -0.15271 | C | -0.59340 | -4.57937 | -1.32354 | C | 0.61468  | -3.43465 | 3.30069  |
| C                      | -6.22468 | -2.43754 | -0.89067 | C | -1.82946 | -4.71640 | -0.62184 | C | 1.85340  | -3.87180 | 2.74224  |
| C                      | -5.78349 | -2.56751 | -2.26527 | C | -3.07162 | -4.59326 | -1.32668 | C | 3.09360  | -3.42484 | 3.30604  |
| C                      | -5.84283 | -3.80406 | -2.96858 | C | -4.28871 | -4.80206 | -0.64850 | C | 4.31429  | -3.91379 | 2.79955  |
| C                      | -4.93642 | -4.10059 | -3.95149 | C | -5.48665 | -4.70950 | -1.41340 | C | 5.50988  | -3.46613 | 3.43006  |
| C                      | -3.90634 | -3.18150 | -4.30089 | C | -5.48719 | -4.12960 | -2.65406 | C | 5.50261  | -2.37857 | 4.26254  |
| O                      | 7.45602  | -0.63000 | -1.59315 | C | 1.85477  | -1.77617 | -4.37927 | C | -3.10138 | -0.27685 | 4.75165  |
| C                      | 7.54575  | -1.06921 | -0.41880 | C | 1.84822  | -0.41124 | -4.70856 | C | -3.09386 | -1.67781 | 4.45873  |
| O                      | 7.90245  | -0.43549 | 0.60408  | C | 0.62733  | -4.72423 | -0.62969 | C | -1.84709 | -2.31171 | 4.14403  |
| C                      | 7.20613  | -2.57023 | -0.23992 | C | 1.86480  | -4.54805 | -1.32348 | C | -1.84063 | -3.42711 | 3.29134  |
| C                      | 7.12874  | -3.03624 | 1.20643  | C | 1.86324  | -3.95268 | -2.59614 | C | -0.60218 | -3.89299 | 2.75666  |
| H                      | -2.99300 | 7.82213  | -0.31942 | C | 3.10559  | -3.52370 | -3.16965 | C | -0.59745 | -4.53924 | 1.48360  |
| H                      | -2.26745 | 7.60762  | -2.60455 | C | 3.10090  | -2.41751 | -4.07702 | C | 0.62472  | -4.70426 | 0.80050  |
| H                      | -0.88178 | 7.15478  | -4.11236 | C | 4.31559  | -1.80251 | -4.43957 | C | 1.85895  | -4.50826 | 1.49065  |
| H                      | 1.26272  | 6.43115  | -4.93384 | C | 4.30915  | -0.39397 | -4.78234 | C | 3.10437  | -4.69156 | 0.80390  |
| H                      | 3.23533  | 5.74969  | -4.71914 | C | 3.08813  | -0.30791 | -4.73977 | C | 4.31980  | -4.56740 | 1.50566  |
| H                      | 5.17117  | 5.06130  | -3.46473 | C | 3.08017  | 1.70870  | -4.44637 | C | 5.52365  | -4.82459 | -0.59135 |
| H                      | 6.24528  | 4.65957  | -1.71035 | C | 1.83331  | 2.34203  | -4.13140 | C | 5.52089  | -4.80339 | 0.77811  |
| H                      | 6.52719  | 4.52220  | 0.67867  | C | 1.82659  | 3.45663  | -3.27760 | C | -3.08081 | -3.90577 | 2.75476  |
| H                      | 5.87856  | 4.71541  | 2.66087  | C | 0.58804  | 3.92174  | -2.74225 | C | -3.07637 | -4.55100 | 1.47744  |
| H                      | 4.28480  | 5.23986  | 4.38647  | C | 3.10778  | -4.71204 | -0.62719 | C | -1.83110 | -4.69614 | 0.78194  |
| H                      | 2.41898  | 5.87031  | 5.11546  | C | 4.32497  | -4.61012 | -1.32932 | C | -4.29126 | -4.77878 | 0.80101  |
| H                      | 0.15447  | 6.65286  | 4.87769  | C | 4.32391  | -3.99619 | -2.64271 | C | -5.49222 | -4.65965 | 1.55698  |
| H                      | -1.52984 | 7.25015  | 3.78443  | C | 5.52169  | -3.56909 | -3.28295 | C | -5.49642 | -4.04236 | 2.77956  |
| H                      | -2.75366 | 7.70568  | 1.76038  | C | 5.51727  | -2.50965 | -4.15108 | C | -4.30062 | -3.50116 | 3.33193  |
| H                      | -3.08421 | -5.72275 | -5.11836 | C | 4.29364  | 2.38111  | -4.20001 | C | -4.30741 | -2.35036 | 4.21308  |
| H                      | -0.81930 | -6.50438 | -4.88029 | C | 5.49660  | 1.71696  | -4.57272 | C | -5.51042 | -1.68597 | 4.58526  |
| H                      | 0.86276  | -7.10204 | -3.78399 | C | 5.50446  | 0.37650  | -4.85353 | C | -5.51772 | -0.34530 | 4.86488  |
| H                      | 2.08434  | -7.55752 | -1.75868 | C | 4.28682  | 3.53208  | -3.31896 | C | -4.32234 | 0.42524  | 4.79328  |
| H                      | 2.32341  | -7.67433 | 0.32130  | C | 3.06684  | 3.93582  | -2.74122 | C | -4.32875 | 1.83386  | 4.45098  |
| H                      | 1.59558  | -7.46014 | 2.60567  | C | 0.58282  | 4.56691  | -1.46867 | C | -5.53075 | 2.54116  | 4.16367  |
| H                      | 0.20905  | -7.00662 | 4.11350  | C | 1.81639  | 4.72679  | -0.76875 | C | -5.53491 | 3.60058  | 3.29558  |
| H                      | -1.93345 | -6.28254 | 4.93961  | C | 3.06178  | 4.58194  | -1.46423 | C | -4.33716 | 4.02799  | 2.65501  |
| H                      | -3.90595 | -5.59891 | 4.73283  | C | 4.27692  | 4.81046  | -0.78842 | C | -4.33813 | 4.64168  | 1.34179  |
| H                      | -5.84258 | -4.91181 | 3.47863  | C | 5.47784  | 4.69106  | -1.54446 | C | -5.53689 | 4.85599  | 0.60355  |
| H                      | -6.90745 | -4.51582 | 1.71610  | C | 5.48260  | 4.07361  | -2.76703 | C | -5.53450 | 4.83463  | -0.76590 |
| H                      | -7.18559 | -4.38170 | -0.67294 | C | -1.87205 | 4.53529  | -1.47612 | C | -4.33316 | 4.59773  | -1.49291 |
| H                      | -6.54199 | -4.57234 | -2.65848 | C | -0.63862 | 4.73051  | -0.78493 | H | 0.54840  | -1.05638 | 0.53544  |
| H                      | -4.94918 | -5.09365 | -4.38607 | C | -0.64115 | 4.75298  | 0.64277  | N | 0.54408  | -1.21801 | -0.47506 |
| H                      | 6.83326  | -4.08849 | 1.28017  | C | 0.57791  | 4.61036  | 1.33545  | H | 6.42168  | 4.01391  | 3.16955  |
| H                      | 6.40201  | -2.43724 | 1.76324  | C | 1.81388  | 4.74868  | 0.63506  | H | 6.42008  | 5.03419  | 0.98836  |
| H                      | 8.09501  | -2.91252 | 1.70227  | C | 3.05678  | 4.62610  | 1.33930  | H | 6.42481  | 4.99253  | -1.11136 |
| H                      | 7.96876  | -3.14295 | -0.78491 | C | 4.27420  | 4.83462  | 0.66121  | H | 6.43323  | 3.90710  | -3.26067 |
| H                      | 6.26449  | -2.76414 | -0.76790 | C | 0.57881  | 4.00534  | 2.62846  | H | 6.44257  | 2.24488  | -4.53279 |
| Ammonium-concave       |          |          |          | C | 1.81557  | 3.55774  | 3.18257  | H | 6.45668  | -0.11181 | -5.02635 |
| surface of SWCNT, CPCM |          |          |          | C | 3.05757  | 4.01996  | 2.63564  | H | 6.46479  | -2.14838 | -4.53414 |
| C                      | -5.51641 | 2.40966  | -4.25113 | C | 4.27568  | 3.63534  | 3.22999  | H | 6.47242  | -4.01121 | -3.00786 |
| C                      | -4.31364 | 1.69310  | -4.51093 | C | 5.47287  | 4.16205  | 2.66668  | H | 6.47394  | -4.90022 | -1.10730 |
| C                      | -3.10003 | 2.31889  | -4.16328 | C | 5.47219  | 4.74199  | 1.42593  | H | 6.46942  | -4.86238 | 1.29959  |
| C                      | -3.10692 | 3.45533  | -3.29346 | C | -3.11764 | 4.72078  | -0.79079 | H | 6.46138  | -3.91814 | 3.17423  |
| C                      | -4.32769 | 3.94381  | -2.78659 | C | -3.12016 | 4.74321  | 0.64041  | H | 6.44869  | -2.00559 | 4.63789  |
| C                      | -5.52327 | 3.49637  | -3.41761 | C | -1.87694 | 4.57893  | 1.33548  | H | 6.43967  | 0.04673  | 5.05827  |
| C                      | -1.85314 | 1.66700  | -4.43798 | C | -1.87602 | 3.98405  | 2.60714  | H | 6.42805  | 2.38623  | 4.48988  |
| C                      | -1.84595 | 0.29290  | -4.72625 | C | -0.63943 | 3.56486  | 3.18336  | H | -6.47474 | 3.94827  | -3.16134 |
| C                      | -3.08576 | -0.42648 | -4.73903 | C | -0.63531 | 2.45992  | 4.08715  | H | -6.46252 | 2.03711  | -4.62684 |
| C                      | -4.30640 | 0.27402  | -4.80710 | C | 0.58678  | 1.83367  | 4.40371  | H | -6.45318 | -0.01525 | -5.04714 |
| C                      | -3.07971 | -1.81696 | -4.40021 | C | 1.81952  | 2.47153  | 4.07188  | H | -6.44226 | -2.35465 | -4.47852 |
| C                      | -4.29393 | -2.48110 | -4.13549 | C | 3.06540  | 1.84858  | 4.41109  | H | -6.43589 | -3.98183 | -3.15717 |
| C                      | -5.49575 | -1.82909 | -4.53286 | C | 4.27979  | 2.51275  | 4.14703  | H | -6.43446 | -5.00211 | -0.97607 |
| C                      | -5.50170 | -0.49849 | -4.85654 | C | 0.59328  | 0.44627  | 4.74053  | H | -6.43925 | -4.96074 | 1.12387  |
| C                      | -1.83393 | -2.43989 | -4.06081 | C | 1.83221  | -0.26194 | 4.73655  | H | -6.44698 | -3.87559 | 3.27322  |
| C                      | -0.60076 | -1.80306 | -4.39503 | C | 3.07202  | 0.45779  | 4.74911  | H | -6.45647 | -2.21375 | 4.54578  |
| C                      | -0.60704 | -0.41536 | -4.73107 | C | 4.29280  | -0.24257 | 4.81802  | H | -6.46986 | 0.14336  | 5.03728  |
| C                      | 0.60922  | 0.29636  | -4.73932 | C | 5.48811  | 0.52980  | 4.86765  | H | -6.47815 | 2.18009  | 4.54728  |
| C                      | 0.60173  | 1.69373  | -4.44647 | C | 5.48159  | 1.86047  | 4.54408  | H | -6.48569 | 4.04306  | 3.02088  |
| C                      | -0.62138 | 2.32967  | -4.15419 | C | -3.11808 | 3.55587  | 3.18109  | H | -6.48720 | 4.93195  | 1.11961  |
| C                      | -0.62838 | 3.46375  | -3.28711 | C | -3.11401 | 2.44848  | 4.08744  | H | -6.48300 | 4.89400  | -1.28747 |
| C                      | -1.86686 | 3.90145  | -2.72899 | C | -1.86793 | 1.80628  | 4.38763  | H | -0.30325 | -0.81102 | -0.87880 |
| C                      | -1.83086 | -3.52535 | -3.17085 | C | -1.86161 | 0.44209  | 4.71955  | H | 1.36793  | -0.77693 | -0.89106 |
|                        |          |          |          | C | -0.62282 | -0.26559 | 4.75050  | H | 0.56259  | -2.22729 | -0.65551 |

# Ammonium-graphene, CPCM

C 7.17328 4.40310 -0.08076  
C 5.73189 4.42504 -0.08567  
C 5.01154 3.19982 -0.08032  
C 5.71837 1.96900 -0.07080  
C 7.15885 1.97059 -0.06520  
C 7.85380 3.23617 -0.07071  
C 5.01004 0.74979 -0.06662  
C 5.72065 -0.47956 -0.05699  
C 7.15772 -0.46758 -0.05002  
C 7.84099 0.77612 -0.05478  
C 5.02337 -1.70648 -0.05364  
C 3.58531 -1.70924 -0.06025  
C 2.87441 -0.49312 -0.06854  
C 3.57758 0.74990 -0.07320  
C 2.87210 1.96921 -0.08065  
C 3.58686 3.20681 -0.08454  
C 5.74585 -2.92691 -0.04279  
C 7.17769 -2.90366 -0.03355  
C 7.85121 -1.67454 -0.03815  
C 2.88234 -2.95060 -0.05753  
C 3.59716 -4.17990 -0.05225  
C 5.06252 -4.17904 -0.03932  
C 5.81197 -5.34843 -0.02185  
C 7.21889 -5.32272 -0.01232  
C 7.89416 -4.12908 -0.01895  
C 1.44134 -0.49481 -0.07789  
C 0.73615 -1.71623 -0.07031  
C 1.45425 -2.95206 -0.06289  
C 0.75007 -4.18360 -0.06077  
C 1.48476 -5.37094 -0.06604  
C 2.86769 -5.36828 -0.06189  
C 1.43873 1.96890 -0.08897  
C 0.73408 0.74572 -0.08539  
C -0.69896 -1.71874 -0.07763  
C -1.41502 -2.95583 -0.06684  
C -0.70793 -4.18559 -0.05596  
C -1.40762 -0.49930 -0.08334  
C -0.70057 0.74402 -0.09679  
C -2.84123 -0.50004 -0.08518  
C -3.54918 -1.71757 -0.07569  
C -2.84318 -2.95725 -0.06852  
C -3.55523 -4.18798 -0.05798  
C -2.82289 -5.37453 -0.03772  
C -1.43998 -5.37446 -0.03648  
C 2.89359 4.44321 -0.09237  
C 1.43579 4.43961 -0.09259  
C 0.72736 3.20767 -0.09198  
C -0.70140 3.20705 -0.09543  
C -1.41054 1.96691 -0.09160  
C -2.84443 1.96320 -0.09317  
C -3.54684 0.74196 -0.08595  
C -4.97935 0.73866 -0.08693  
C -5.68720 -0.49243 -0.08176  
C -4.98722 -1.71790 -0.07633  
C -5.70703 -2.94000 -0.07210  
C -5.02074 -4.19069 -0.06591  
C -7.12439 -0.48374 -0.08352  
C -7.81526 -1.69221 -0.08088  
C -7.13904 -2.91985 -0.07588  
C -7.85256 -4.14713 -0.07560  
C -7.17446 -5.33915 -0.07342  
C -5.76743 -5.36191 -0.06922  
C -7.81003 0.75874 -0.08896  
C -7.13057 1.95473 -0.09262  
C -5.69010 1.95649 -0.09122  
C -4.98614 3.18890 -0.09556  
C -3.56155 3.19939 -0.09412  
C -2.87075 4.43728 -0.09783  
C -1.41290 4.43708 -0.09495  
C -0.68018 5.62684 -0.09216  
C 0.70058 5.62794 -0.09106  
C -5.70915 4.41262 -0.10070

C -7.15048 4.38737 -0.10211  
C -7.82830 3.21883 -0.09831  
C -5.00016 5.61469 -0.10512  
C -3.61581 5.62541 -0.10385  
C 5.02034 5.62563 -0.09615  
C 3.63604 5.63306 -0.09948  
H -1.21772 -0.04674 3.62673  
N -0.73065 0.78852 3.29485  
H -7.67827 5.33652 -0.10668  
H 7.69890 5.35346 -0.08523  
H -8.90200 -1.68530 -0.08319  
H -8.89686 0.75541 -0.09019  
H -8.91402 3.20280 -0.09952  
H -8.93794 -4.12065 -0.07844  
H -7.71828 -6.27777 -0.07528  
H -5.27783 -6.32783 -0.07010  
H -3.32814 -6.33198 -0.02021  
H -0.93694 -6.33240 -0.01680  
H 0.98369 -6.33007 -0.07598  
H 3.37496 -6.32479 -0.06763  
H 5.32449 -6.31541 -0.01342  
H 7.76469 -6.26007 0.00081  
H 8.97945 -4.09997 -0.01194  
H 8.93794 -1.66526 -0.03191  
H 8.92782 0.77503 -0.05013  
H 8.93954 3.22259 -0.06683  
H -5.54715 6.55274 -0.11025  
H -3.11597 6.58558 -0.10858  
H -1.18533 6.58402 -0.08990  
H 1.20395 6.58605 -0.08725  
H 3.13409 6.59210 -0.10910  
H 5.56526 6.56487 -0.10169  
H -1.21816 1.62278 3.62860  
H 0.22766 0.78834 3.65035  
H -0.71431 0.78991 2.26920

## Ammonium-convex surface of SWCNT, CPCM

C -5.54288 1.11745 4.69320  
C -4.36861 1.84950 4.35696  
C -3.12861 1.21253 4.56302  
C -3.07945 -0.20231 4.77399  
C -4.27164 -0.95379 4.77546  
C -5.49578 -0.23643 4.89602  
C -1.90849 1.91202 4.28458  
C -1.94788 3.07332 3.49599  
C -3.20744 3.53125 2.98705  
C -4.40915 3.04747 3.54173  
C -3.23187 4.24392 1.74620  
C -4.45667 4.46218 1.08480  
C -5.64963 4.25495 1.83381  
C -5.62657 3.57155 3.02075  
C -1.99539 4.47232 1.05778  
C -0.75357 4.32359 1.74642  
C -0.72994 3.61464 2.98538  
C 0.50545 3.17585 3.50226  
C 0.54526 1.99567 4.30504  
C -0.65109 1.29574 4.56017  
C -0.60213 -0.11569 4.76980  
C -1.81243 -0.86869 4.69755  
C -2.00020 4.57408 -0.34313  
C -3.23939 4.44522 -1.05264  
C -4.46064 4.56781 -0.36124  
C 0.45872 4.57190 1.07220  
C 0.45592 4.67546 -0.35399  
C -0.76142 4.52386 -1.05345  
C -0.74290 3.99731 -2.38102  
C -1.96367 3.53543 -2.95717  
C -3.22069 3.91579 -2.38170  
C -4.42512 3.51926 -2.99556  
C -5.63952 3.96571 -2.40036  
C -5.65696 4.47234 -1.12802  
C 1.70157 4.38983 1.74876  
C 1.72424 3.69108 2.96647  
C 0.48965 3.63716 -2.95979

C 1.71213 4.07017 -2.36176  
C 1.69636 4.59029 -1.05862  
C 2.93355 4.76358 -0.35602  
C 2.93614 4.66112 1.07213  
C 4.15757 4.54783 1.76495  
C 4.18160 3.82647 3.02205  
C 2.98276 3.26405 3.50394  
C 3.02246 2.08113 4.30870  
C 1.80292 1.36627 4.54724  
C 1.85105 -0.02194 4.75242  
C 0.64077 -0.77759 4.71507  
C 2.96743 3.72761 -2.96287  
C 4.16912 4.21524 -2.41103  
C 4.15161 4.74948 -1.06396  
C 5.34379 4.96759 -0.31596  
C 5.34648 4.87013 1.04997  
C 4.26070 1.48398 4.61627  
C 5.43395 2.26007 4.39545  
C 5.39608 3.39180 3.62540  
C 4.31063 0.05081 4.82792  
C 3.11813 -0.69183 4.71811  
C 0.68807 -2.14031 4.29241  
C 1.94350 -2.70697 3.91880  
C 3.16562 -2.05789 4.29401  
C 4.40394 -2.65609 3.98718  
C 5.58074 -1.98201 4.42127  
C 5.53562 -0.67489 4.82751  
C -1.76597 -2.20879 4.28185  
C -0.50990 -2.79319 3.93919  
C -0.47443 -3.83993 2.96916  
C 0.75760 -4.19764 2.38666  
C 1.97828 -3.73652 2.96503  
C 3.23508 -4.11644 2.38950  
C 4.43989 -3.72089 3.00392  
C 0.77532 -4.72602 1.06089  
C 2.01305 -4.77713 0.35215  
C 3.25267 -4.64664 1.06068  
C 4.47469 -4.76985 0.37013  
C 5.67098 -4.67486 1.13696  
C 5.65416 -4.16795 2.40924  
C -2.98716 -2.88002 3.94453  
C -2.95158 -3.92903 2.97172  
C -1.69607 -4.27157 2.37057  
C -1.67876 -4.79045 1.06638  
C -0.43978 -4.87657 0.36299  
C -0.44327 -4.77555 -1.06134  
C 0.76858 -4.52865 -1.73710  
C 2.00972 -4.67789 -1.04854  
C 3.24613 -4.44768 -1.73677  
C 4.47130 -4.66506 -1.07579  
C 0.74493 -3.81739 -2.97494  
C 1.96286 -3.27582 -3.48600  
C 3.22242 -3.73421 -2.97736  
C 4.42424 -3.25050 -3.53224  
C 5.64192 -3.77455 -3.01174  
C 5.66444 -4.45755 -1.82465  
C -2.91716 -4.96356 0.36499  
C -2.92061 -4.86203 -1.06294  
C -1.68565 -4.59212 -1.73919  
C -1.70888 -3.89375 -2.95722  
C -0.49015 -3.37867 -3.49288  
C -0.52994 -2.19763 -4.29454  
C 0.66637 -1.49786 -4.55021  
C 1.92358 -2.11428 -4.27434  
C 3.14367 -1.41496 -4.55280  
C 4.38360 -2.05194 -4.34654  
C 0.61739 -0.08637 -4.75895  
C 1.82793 0.66662 -4.68712  
C 3.09486 0.00001 -4.76331  
C 4.28709 0.75146 -4.76516  
C 5.51128 0.03411 -4.88557  
C 5.55793 -1.31974 -4.68270  
C -2.96731 -3.46656 -3.49485  
C -3.00719 -2.28328 -4.29915  
C -1.78753 -1.56826 -4.53733

|   |          |          |          |   |          |          |          |   |          |          |          |
|---|----------|----------|----------|---|----------|----------|----------|---|----------|----------|----------|
| C | -1.83569 | -0.18004 | -4.74283 | C | -3.15061 | 1.85567  | -4.28491 | C | -4.14238 | -4.74966 | -1.75587 |
| C | -0.62554 | 0.57553  | -4.70579 | C | -1.92845 | 2.50519  | -3.91019 | C | -5.33099 | -5.07196 | -1.04094 |
| C | -0.67291 | 1.93816  | -4.28252 | C | -4.38893 | 2.45429  | -3.97893 | C | -5.32764 | -5.16922 | 0.32519  |
| C | 0.52529  | 2.59141  | -3.93046 | C | -5.56561 | 1.78009  | -4.41263 | C | -4.13551 | -4.95044 | 1.07274  |
| C | 1.78151  | 2.00682  | -4.27208 | C | -5.52009 | 0.47272  | -4.81829 | C | -4.15343 | -4.41629 | 2.42007  |
| C | 3.00259  | 2.67824  | -3.93532 | C | -4.29523 | -0.25302 | -4.81847 | C | -5.36422 | -4.07688 | 3.08799  |
| C | 4.23902  | 2.13547  | -4.33757 | C | -4.24540 | -1.68636 | -4.60745 | C | -5.39819 | -3.07297 | 4.01902  |
| C | 5.37997  | 3.87557  | -3.07892 | C | -5.41875 | -2.46237 | -4.38713 | C | -4.22370 | -2.33787 | 4.34775  |
| C | 5.41351  | 2.87096  | -4.00905 | C | -5.38072 | -3.59393 | -3.61683 |   |          |          |          |
| C | -3.10276 | 0.48971  | -4.70892 | C | -4.16640 | -4.02855 | -3.01306 |   |          |          |          |
| H | -0.93106 | 8.03459  | 0.60035  | H | 6.37302  | 2.57050  | -4.41428 | H | -6.53246 | 2.26202  | -4.32363 |
| N | -0.59948 | 7.97604  | -0.36498 | H | 6.44283  | 0.56778  | -5.03519 | H | -6.45235 | -0.03536 | -5.03702 |
| H | 6.62779  | -4.90315 | 0.68115  | H | 6.52429  | -1.81107 | -4.67690 | H | -6.37970 | -2.10567 | -4.73974 |
| H | 6.59870  | -4.01452 | 2.91855  | H | 6.58352  | -3.54348 | -3.49669 | H | -6.31317 | -4.09539 | -3.38406 |
| H | 6.54748  | -2.46416 | 4.33209  | H | 6.62336  | -4.74544 | -1.40902 | H | -6.27840 | -5.13937 | -1.56351 |
| H | 6.46791  | -0.16699 | 5.04655  | H | -6.42726 | -0.77028 | 5.04554  | H | -6.27270 | -5.31018 | 0.83701  |
| H | 6.39496  | 1.90320  | 4.74771  | H | -6.50935 | 1.60856  | 4.68736  | H | -6.29800 | -4.53877 | 2.78805  |
| H | 6.32854  | 3.89314  | 3.39258  | H | -6.56819 | 3.34034  | 3.50559  | H | -6.35777 | -2.77280 | 4.42430  |
| H | 6.29370  | 4.93730  | 1.57286  | H | -6.60863 | 4.54281  | 1.41849  | H | -1.34057 | 8.27992  | -0.99998 |
| H | 6.28902  | 5.10829  | -0.82745 | H | -6.61392 | 4.69979  | -0.67223 | H | 0.21848  | 8.57781  | -0.48233 |
| H | 6.31376  | 4.33766  | -2.77944 | H | -6.58398 | 3.81177  | -2.90962 | H | -0.34259 | 7.00573  | -0.57913 |