

Supporting information

Confined Platinum Nanoparticle in Carbon Nanotube: Structure and Oxidation

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SSW Method

The SSW algorithm^{1,2} features with an automated climbing mechanism to manipulate one minimum to a high energy configuration along one random direction, which is inherited from the bias-potential driven constrained-Broyden-dimer (BP-CBD) method for TS location developed in the group³. The method has been successfully utilized for predicting the structure of finite clusters with complex PES, such as C₁₀₀ fullerene, and the detail of the algorithm can be found in our previous papers^{1,2}. Here we briefly outline the central idea of the SSW method and an illustration of the SSW method is shown in Figure S1.

In one particular SSW step, labeled as i , a modified PES V_{m-to-H} , as shown in Eq. S1, is utilized for moving from the current minimum, \mathbf{R}_i^m to a high energy configuration \mathbf{R}_i^H , in which a series of bias Gaussian potential v_n (n is the index of the bias potential, $n=1,2,\dots,H$) is added one by one consecutively along the direction \mathbf{N}_i^n .

$$V_{m-to-H} = V_{real} + \sum_{n=1}^H v_n = V_{real} + \sum_{n=1}^H w_n \times \exp \left[-\frac{((\mathbf{R}^t - \mathbf{R}_i^{n-1}) \cdot \mathbf{N}_i^n)^2}{2 \times ds^2} \right] \quad (\text{S1})$$

$$\mathbf{F}_{tot} = \mathbf{F}_{real} + \sum_n w_n \cdot \exp \left[-\frac{((\mathbf{R}^t - \mathbf{R}_i^{n-1}) \cdot \mathbf{N}_i^n)^2}{2 \times ds^2} \right] \cdot \frac{(\mathbf{R}^t - \mathbf{R}_i^{n-1}) \cdot \mathbf{N}_i^n}{ds^2} \cdot \mathbf{N}_i^n \quad (\text{S2})$$

where \mathbf{R} is the coordination vector of the structure and V_{real} represents the unmodified PES; \mathbf{R}_i^n are the n^{th} local minima along the movement trajectory on the modified PES that is created after adding n Gaussian functions (see Figure S1). The PES at \mathbf{R}_i^n is thus defined by $V_{m-to-n} = V_{real} + \sum_{k=1}^n v_k$. The Gaussian function is controlled by its height w and its width ds , and is always added along one particular walking direction as defined by \mathbf{N}^n .

\mathbf{N}^n should desirably be one eigenstate of Hessian matrix (normal mode) with low eigenvalues. Since the computation of Hessian is expensive, SSW method optimizes \mathbf{N}^n iteratively from the initial random direction \mathbf{N}^0 using the biased CBD rotation method^{1,3}, which is utilized practically to fast locate one soft eigenvector of Hessian matrix. It should be noticed that as inherited from CBD rotation⁴, the biased CBD rotation does not compute the whole Hessian matrix but aims to find one vector close to a soft eigenvector of Hessian using the numerical approach. Owing to the extra bias added in the CBD rotation^{5,6}, the biased CBD rotation distinguishes from other existing eigenvector updating schemes as utilized in single-ended TS searching method like dimer⁷, CBD⁴, hybrid eigenvector-following⁸ and

GAD^{9, 10}, the rotation does not necessarily converges to the softest eigenvector or even any eigenvector of Hessian exactly, but to a vector that mimics the initial random direction \mathbf{N}^0 and at the meantime is close to a soft eigenvector of Hessian. In short, the biased CBD method is able to follow up one particular moving direction to escape the basin region, which is not always the softest mode direction (e.g. frustrated translational/rotational modes). More details on the random mode generation and optimization can be found in our previous works.^{1, 3}

Overall, the movement from \mathbf{R}_i^m to \mathbf{R}_i^H (see Figure S1) is a repeated procedure containing (i) the update of the direction \mathbf{N}_i^n at \mathbf{R}_i^{n-1} ; (ii) the adding of a new Gaussian function v_n and the displacement of \mathbf{R}_i^{n-1} along the direction \mathbf{N}_i^n by a magnitude of $ds (\mathbf{R}_i^{n-1} + \mathbf{N}_i^n \cdot ds)$; and (iii) the local relaxation to \mathbf{R}_i^n on the modified PES (the energy minimization is constrained by the added potentials). The force for the local optimization on the modified PES can be evaluated according to Eq. S2. After reaching the high energy structure \mathbf{R}_i^H , we remove all the added bias potentials and relax fully until a new minimum is found.

It might be noticed that the purpose of adding bias potential in SSW method is quite different from the MD-based metadynamics⁶ method. In SSW method, the bias potential is for driving the structure across the TS and will be removed before the full energy minimization. In metadynamics, the bias potentials are kept during the simulation to gradually fill the basins. Special reaction coordinate, i.e. collective variables, needs to be designed in order to fill only those related basins and drive the simulation to the target state. In contrast, the bias potential in SSW method is imposed simply using the Cartesian coordinate, the direction of which is obtained from the biased CBD rotation. There is no need for guessing the reaction coordinate.

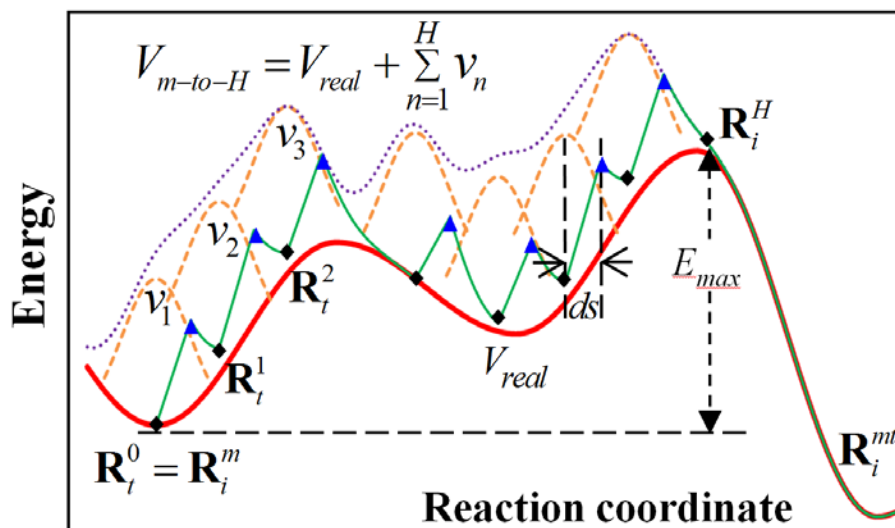


Figure S1. The illustration of the SSW method. The real PES is described by the red curve showing separated minima. one SSW step from one minimum to another, where the bias Gaussian potentials are imposed only on the atom degrees of freedom^{1,2}. The green curve represents the subsequent atom relaxation.

The detail of the force field and the comparison with the DFT on the Pt₁₅ system

Semi-empirical potentials such as the many-body Sutton-Chen (SC)¹¹ and the embedded-atom method¹² are popular choices for the face centered cubic (fcc) and other close-packed metal clusters. Such potential models include the effect of the local electron density to account for many-body terms. The SC potential chosen to describe the Pt-Pt interactions provides reasonable descriptions of bulk and small cluster properties of metal and metal alloys¹³⁻¹⁸. The potential energy in the SC model can be expressed by

$$U_{tot} = \varepsilon \left[\frac{1}{2} \sum_{i \neq j} \sum \left(\frac{a}{r_{ij}} \right)^n - c \sum_i \rho_i^{1/2} \right] \quad (\text{S3})$$

The first term in equation (S3) is a pair-wise repulsive potential and the second one represents the metallic bonding energy associated with ρ_i , the local electron density, defined as

$$\rho_i = \sum_{i \neq j} \left(\frac{a}{r_{ij}} \right)^m \quad (\text{S4})$$

where r_{ij} is the distance between atoms i and j , c is a dimensionless parameter, ε is a parameter with the dimensions of energy, and a is a length parameter. For the description of the Pt-Pt interaction, the adopted the values are $\varepsilon = 0.019833$ eV, $a = 3.92$ Å, $c = 34.408$, $m = 8$, and $n = 10$ ¹¹,¹⁸, which has been utilized previously in the study of Pt nanoparticle deposited on the graphite substrate¹⁹,

Following the previous work^{19,20}, we employ a 12-6 Lennard-Jones potential²¹ to describe metal-carbon interactions. This approximation is expected to capture the essential physics of the system and to yield a qualitatively correct description. Quantitative details, however, could only be obtained with a more precise description of metal-carbon interactions. The Lennard-Jones parameters used here are $\sigma = 2.90$ Å and $\epsilon = 0.0220$ eV.^{19,20} These are derived

by fitting the Lennard-Jones potential to simulation data for platinum obtained using a many-body potential (the Sutton-Chen potential¹¹) to obtain Pt-Pt parameters, then using Lorentz-Berthelot mixing rules²¹ to determine Pt-C parameters. The cutoff distance for the Pt-C interactions is set to 12.0 Å.

To confirm the validity of the force field (SC/LJ) calculations, several properties of the Pt₁₅ system were calculated by both DFT and the force field. The DOS-m for Pt₁₅ inside and outside CNT are shown in Figure S2a, providing an 1-D overview for the PES of the supported Pt particles. The largest peak in DOS-m of SC/LJ methods shifts downwards in energy for Pt@CNT compared to that for Pt/CNT, which is consistent with the DFT results. The Pt-Pt distance distribution function inside and outside CNT from the minima collected from SSW trajectories are plotted in Figure S2b. The shortest Pt-Pt bond length in the results of DFT and SC/LJ methods agree in a small window of 2.64~2.70 Å. Although the GS structure obtained from DFT and SC/LJ method are different, the similar attenuation of the $\sqrt{2}a$ ($a=2.7$ Å) peak and amplification of the $\sqrt{3}a$ peak can be observed for Pt₁₅ cluster inside CNT. The adsorption energy (ΔE) for adding a Pt₁₅ cluster into the CNT can be found in Table S1. We found that ΔE from force field calculations are generally very close to the DFT results, no matter using the GS structure of DFT or using the GS structure of the SC/LJ methods. These comparisons show that the SC/LJ results can yield a qualitatively correct description for Pt nanoparticles interacting with CNT.

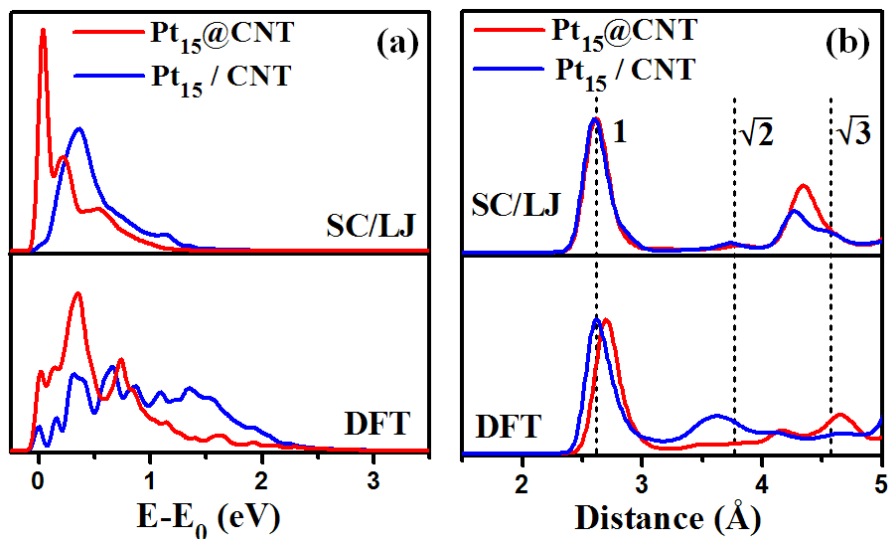


Figure S2. The comparison between the results of DFT and force field methods for Pt₁₅ cluster inside and outside CNT. All the minima are from SSW trajectories at 5000 K. (a) The density of the states of minima (DOS-m). (b) The Pt-Pt distance distribution. For comparison, each plot is normalized according to the area of the first Pt-Pt distance peak at ~ 2.7 Å that corresponds to the shortest Pt-Pt bond length.

Table S1. The adsorption energy of Pt₁₅ inside CNT (Pt₁₅@CNT)

	ΔE (eV)
DFT	-3.87
SC/LJ (using DFT GS structure)	-3.70
SC/LJ (using its own GS structure)	-3.93

The coordination number of the Pt atoms for Pt₁₅@CNT and Pt₁₅/CNT

By counting the number of Pt-Pt and Pt-C pairs with Pt-Pt distance less than 3.1 Å and Pt-C distance less than 2.8 Å, we have determined the coordination number of the Pt atoms for the GS of Pt₁₅@CNT and Pt₁₅/CNT, as shown in Figure S3. It is found that the number of low coordination Pt atoms (the coordination number in the range of 3~6) in Pt₁₅/CNT (11 atoms) are much more than that in Pt₁₅@CNT (5 atoms). The Pt atoms at the terminal sites are generally low coordinated, and these sites are critical for catalytic reactions, as shown in this work for O₂ adsorption and dissociation.

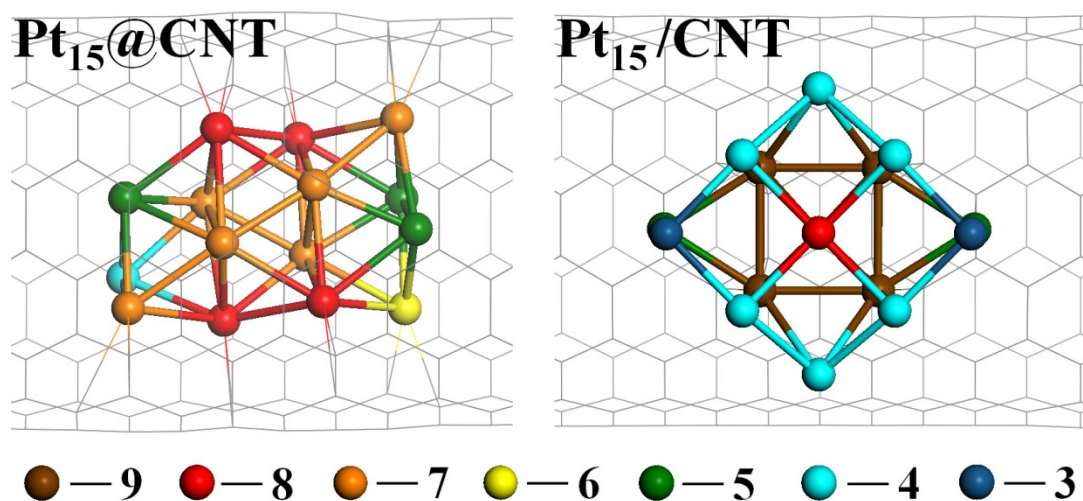


Figure S3. The coordination number of Pt in the GS of Pt₁₅@CNT and Pt₁₅/CNT. The coordination takes into account of the first neighbors of Pt, including those with Pt-Pt bond below 3.1 and Pt-C bond below 2.8 Å.

Pt-C distance for CNT supported Pt₁₅@CNT and Pt₁₅/CNT

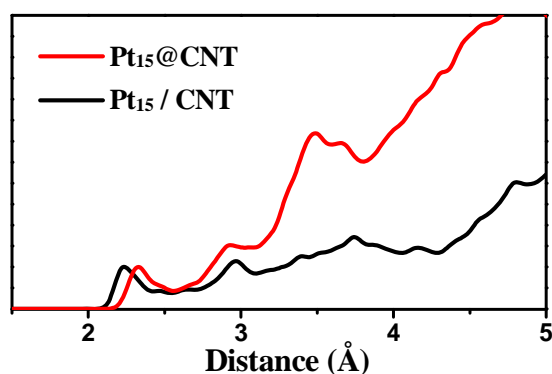


Figure S4. The Pt-C distance distribution for the Pt₁₅ inside and outside the CNT statistically averaged from all the minima obtained from SSW trajectories at 5000 K.

As shown, the shortest Pt-C distance is 2.2~2.4 Å, which is consistent with the previous reports²² for Pt clusters supported on graphene. From the distance, the bond order of Pt-C bond can be characterized as single bond, e.g. the typical single Pt-C bond is 2.08 and 1.98 Å for sp³ and sp² carbons, respectively²³. The number of Pt-C bond in Pt₁₅@CNT is in general larger than that in Pt₁₅/CNT, also shown in the following Table S2.

Table S2. The numbers of the Pt-C bond (below 2.8 Å, N_{Pt-C}) and the Bader charge (Q) for the GS of CNT supported Pt₁₅.

	Inside CNT	Outside CNT
N _{Pt-C}	19	16
Q _{Pt} (e)	0.61	0.59

O₂ adsorption on CNT supported Pt₁₅ and Pt₁₅O₄

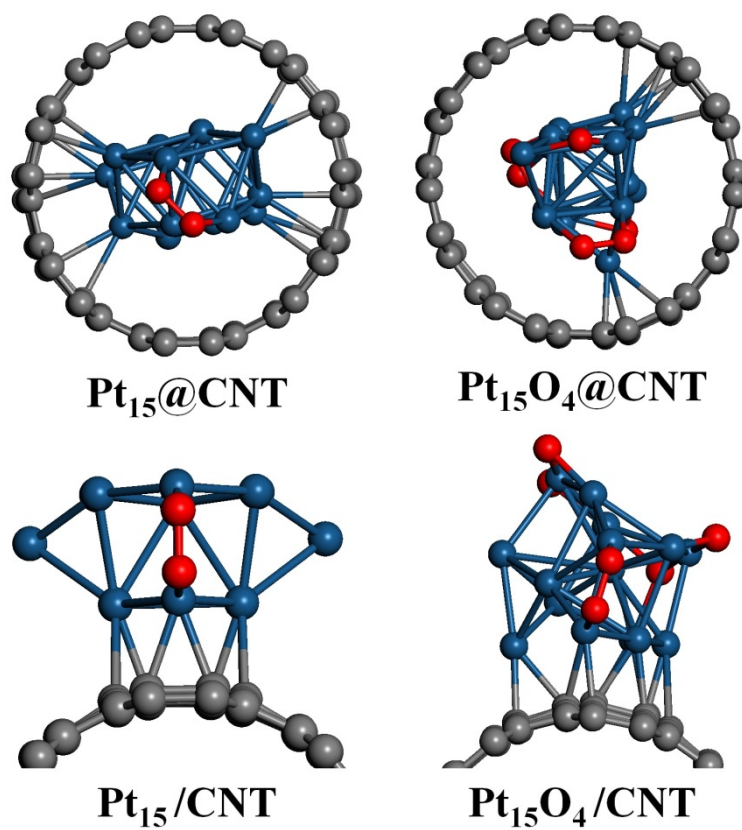


Figure S5. The most stable structures of O₂ adsorbed on CNT supported Pt₁₅ and Pt₁₅O₄.

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The XYZ coordinates for the GSs of Pt₁₅, Pt₁₅O₂, Pt₁₅O₄ and Pt₁₅O₆ particles at both sides of CNT

Pt₁₅/CNT: (in total 351 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
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C	12.938403	11.484582	3.415706
C	11.913471	12.492847	3.416912
C	9.305453	13.664848	3.419507
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C	7.871802	13.710641	13.189191
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Pt	15.746277	9.137583	4.490663
Pt	18.270137	9.325063	7.699695
Pt	15.735877	9.133717	7.282083

Pt	16.063914	14.158975	5.893817
Pt	15.083620	11.956298	7.279172
Pt	17.457813	12.892775	4.101801
Pt	17.644304	11.059154	5.900613
Pt	18.284625	9.329079	4.102730
Pt	15.499004	10.568374	9.553119
Pt	17.583593	7.581688	5.895860
Pt	18.017408	11.146697	9.499395
Pt	15.515406	10.567347	2.213143
Pt	18.031957	11.147743	2.300845

Pt₁₅@CNT(in total 351 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma) 28.0000 28.0000 29.3063

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C	4.474995	11.264578	0.978225
C	3.879406	8.474285	0.972847
C	4.207088	7.079157	0.972302
C	5.986009	4.849940	0.977244
C	7.278139	4.230251	0.980096
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C	5.427202	5.319201	21.741281
C	7.190385	13.509422	21.744466
C	5.909407	12.868563	21.743713
C	8.008502	4.109706	21.738438
C	9.441244	4.132371	21.739492
C	11.337770	12.930925	21.751628
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C	11.991046	5.410040	21.748383
C	12.871873	6.540521	21.753243
C	4.171409	10.608414	21.744781
C	13.476461	8.599097	22.978176
C	12.812483	11.373654	22.976552
C	11.908599	12.485630	22.973499
C	9.328335	13.699725	22.966811
C	7.895602	13.684776	22.965370
C	5.348580	12.406678	22.964698
C	4.477619	11.269169	22.964687
C	3.880724	8.479656	22.964703
C	4.208886	7.085018	22.963869
C	6.000009	4.866583	22.959956
C	7.296333	4.256097	22.959195
C	10.145918	4.299134	22.962544
C	11.425888	4.943988	22.966687
C	13.173660	7.198171	22.976402
C	3.877685	9.206785	24.184470
C	13.458758	9.326777	24.198400
C	13.127588	10.720870	24.197682
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C	10.037449	13.549850	24.188504
C	11.982488	5.403753	24.190955
C	12.858329	6.538220	24.194530
C	4.176630	10.607583	24.184889
C	13.457068	8.599028	25.418482
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C	11.902762	12.491765	25.413121
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C	7.892645	13.694068	25.406882
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C	3.888065	8.478127	25.403420
C	4.214992	7.083663	25.402642
C	5.998275	4.858633	25.400810
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C	11.418174	4.936226	25.409518
C	13.156200	7.198237	25.417305
C	3.882279	9.205316	26.622817
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C	7.999758	4.082205	26.623132
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C	7.286289	4.233758	27.843413
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C	11.409164	4.931804	27.852394
C	13.137417	7.201036	27.857326
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C	10.035061	13.566368	29.072084

C	11.960549	5.400491	29.075557
C	12.826021	6.542036	29.076621
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Pt	9.979549	7.776953	13.349126
Pt	10.705689	10.374173	13.232547
Pt	8.107016	7.357680	6.757105
Pt	8.835084	9.985814	6.418960
Pt	6.461715	9.811193	11.128891
Pt	7.800502	10.068739	8.826720
Pt	10.708398	8.105899	6.680451
Pt	6.698328	7.644029	9.203579
Pt	10.542557	10.171409	8.620246
Pt	8.102756	9.668936	13.305138
Pt	9.157511	10.512476	11.004204
Pt	6.221323	9.215477	6.868673
Pt	10.980662	8.666767	10.965581
Pt	8.205305	7.725676	11.379700
Pt	9.443539	7.730636	9.031289

Pt₁₅O₂/CNT: (in total 353 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
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C	9.301610	13.756061	15.633322
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C	4.476212	11.269235	15.635970
C	3.892572	8.476854	15.635212
C	4.215316	7.081305	15.635089
C	5.983977	4.845502	15.635224
C	7.275060	4.224209	15.634416
C	10.122115	4.269331	15.632235
C	11.391225	4.933779	15.631270
C	13.079709	7.227354	15.635550
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C	13.365683	9.353239	16.857235
C	13.061215	10.750971	16.860226
C	4.528417	6.425063	16.856247
C	5.417613	5.301934	16.856315
C	7.164273	13.544871	16.855560
C	5.893093	12.883793	16.856468
C	7.986290	4.068555	16.855488
C	9.418942	4.089261	16.854530
C	11.305973	12.994590	16.858234
C	10.011597	13.608192	16.856658
C	11.944473	5.404302	16.852930
C	12.792613	6.558051	16.854146
C	4.177028	10.605889	16.856632
C	13.381540	8.622839	18.074322
C	12.754095	11.408189	18.079520
C	11.871778	12.536034	18.078970
C	9.300072	13.759081	18.077914
C	7.867736	13.726761	18.077706
C	5.338407	12.412463	18.077606
C	4.476537	11.268008	18.077780

C	3.888934	8.476148	18.077093
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C	7.277181	4.227749	18.077183
C	10.124973	4.268270	18.075474
C	11.395814	4.929476	18.074520
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C	3.879693	9.203304	19.298059
C	13.384026	9.349187	19.293795
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C	4.526697	6.425045	19.298304
C	5.418263	5.303543	19.298367
C	7.163459	13.543520	19.299099
C	5.892446	12.882299	19.299059
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C	10.010660	13.604040	19.299814
C	11.950578	5.403251	19.294382
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C	12.756868	11.401391	20.516359
C	11.870760	12.526665	20.518281
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C	5.337172	12.411127	20.519757
C	4.474527	11.267370	20.519524
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C	11.400069	4.932084	20.516802
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C	13.396661	9.345994	21.731490
C	13.074028	10.741812	21.733430
C	4.525830	6.425779	21.740251
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C	7.990848	4.078241	21.740102
C	9.423444	4.099383	21.740169
C	11.303760	12.978208	21.739684
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C	4.172292	10.605154	21.740193
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C	11.873975	12.519808	22.957425
C	9.300965	13.744005	22.963889
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C	5.335564	12.410303	22.961777
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C	9.425084	4.105491	24.182278
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C	11.959781	5.408473	24.178620
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C	5.414277	5.299194	11.971580
C	7.166295	13.528442	11.968752
C	5.887800	12.881769	11.970832
C	7.981888	4.069107	11.969612
C	9.414193	4.105899	11.968075
C	11.315624	12.962205	11.971353
C	10.015980	13.566315	11.968434
C	11.933052	5.440647	11.970072
C	12.796603	6.584646	11.973799
C	4.171274	10.607353	11.973082
C	13.399152	8.633392	13.205076
C	12.778693	11.413881	13.204647
C	11.883525	12.530998	13.198569
C	9.304361	13.735809	13.188230
C	7.871802	13.710641	13.189191
C	5.333634	12.414581	13.193207
C	4.472018	11.270295	13.193978
C	3.894433	8.477305	13.193256
C	4.217420	7.082156	13.192918
C	5.981422	4.843380	13.192694
C	7.272327	4.222473	13.191758
C	10.119151	4.282860	13.188965
C	11.385911	4.951809	13.187836
C	13.094299	7.234624	13.199597
C	3.885218	9.204327	14.414599
C	13.374972	9.359490	14.423012
C	13.072767	10.755778	14.425849

C	4.529821	6.425598	14.413963
C	5.416397	5.300644	14.414161
C	7.165598	13.539738	14.411768
C	5.891921	12.883558	14.413508
C	7.984264	4.067265	14.412432
C	9.416826	4.093189	14.410745
C	11.309419	12.989155	14.415317
C	10.013445	13.598465	14.412600
C	11.939691	5.413796	14.411366
C	12.789688	6.565449	14.414275
C	4.175952	10.606751	14.415067
O	18.808765	9.448324	9.143926
O	17.868813	13.146358	9.127410
Pt	15.071297	11.947139	4.487854
Pt	17.209724	13.526414	7.334221
Pt	15.728732	9.138759	4.503086
Pt	18.364123	8.768572	7.373227
Pt	15.742037	9.074158	7.324708
Pt	15.300884	14.286004	5.720475
Pt	15.029400	12.048482	7.310432
Pt	17.399811	13.045102	4.567746
Pt	17.482426	11.063184	6.239191
Pt	18.299420	9.230136	4.595018
Pt	15.515711	10.596423	9.512175
Pt	17.010796	7.191374	5.787348
Pt	18.054773	11.225446	9.166129
Pt	15.545831	10.568906	2.260712
Pt	18.005560	11.161223	2.879541

Pt₁₅O₂@CNT: (in total 353 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
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C	12.806179	11.392157	0.999969
C	11.912676	12.511660	1.001169
C	9.330244	13.716825	1.002214
C	7.897039	13.691483	1.000733
C	5.352602	12.404105	0.995635
C	4.480970	11.265980	0.992981
C	3.885381	8.475687	0.987603
C	4.213063	7.080559	0.987058
C	5.991984	4.851342	0.992000
C	7.284114	4.231653	0.994852
C	10.131995	4.277468	1.001904
C	11.405620	4.935503	1.003813
C	13.128887	7.207634	1.004852
C	3.870024	9.202070	2.207040
C	13.437291	9.342234	2.219365
C	13.131629	10.742266	2.219312
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C	7.190260	13.512089	2.220553
C	5.910270	12.866554	2.218320
C	7.989463	4.078206	2.219562
C	9.422298	4.100663	2.221761
C	11.343249	12.959947	2.223628
C	10.041995	13.560000	2.223090

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C	4.170167	10.603478	2.209951
C	13.444707	8.618301	3.438567
C	12.830549	11.405575	3.438781
C	11.921574	12.512693	3.443005
C	9.329860	13.700183	3.444238
C	7.897361	13.681602	3.442077
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C	11.396036	4.939247	3.444815
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C	13.163963	10.755027	4.655991
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C	5.907994	12.869491	4.656688
C	7.980956	4.096369	4.663676
C	9.414289	4.109107	4.665024
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C	5.357718	12.404563	5.877662
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C	13.185092	10.730280	7.095893
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C	7.985157	4.104841	7.108255
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C	11.305616	12.893965	7.103431
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C	11.909693	5.457772	7.108742
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C	12.784093	11.322125	8.332712
C	11.833060	12.401040	8.335578
C	9.337454	13.702092	8.333107
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C	5.353612	12.400208	8.333798
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C	13.145242	7.242569	10.769701
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C	13.264412	10.753489	11.984068
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C	7.211554	13.519845	11.995958
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C	11.422468	5.017272	13.214492
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C	7.998442	4.075928	29.081653
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Pt	11.137887	8.548902	10.930799
Pt	8.545837	7.486253	11.276741
Pt	9.601210	7.817718	8.884183

Pt₁₅O₄/CNT: (in total 355 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
C	10.814511	12.198676	0.982608
C	7.994614	12.581307	0.986599
C	6.633258	12.136978	0.988938
C	4.609512	10.134367	0.989588
C	4.149636	8.777146	0.988130
C	4.514265	5.949870	0.983792
C	5.291704	4.746679	0.982835
C	7.708562	3.230302	0.984356
C	9.130312	3.055919	0.985686
C	11.830997	3.968913	0.990179
C	12.850445	4.975750	0.990661
C	13.788776	7.665619	0.984053
C	13.611829	9.087288	0.979625
C	12.038139	11.460917	0.972978
C	7.019096	3.470931	2.203702

C	10.143147	12.459183	2.201314
C	8.722854	12.644097	2.203511
C	9.850562	3.129764	2.208222
C	11.206866	3.591075	2.210802
C	4.078466	8.051085	2.208770
C	4.260540	6.629734	2.206193
C	13.229662	5.599013	2.212747
C	13.702672	6.951609	2.210718
C	6.018436	11.753737	2.211751
C	4.998735	10.746979	2.212900
C	13.369303	9.780362	2.194903
C	12.583839	10.976982	2.188193
C	5.805691	4.232085	2.203450
C	10.848329	12.238791	3.408171
C	8.008077	12.572048	3.426029
C	6.648887	12.124690	3.430974
C	4.620695	10.125977	3.434836
C	4.154224	8.771262	3.432756
C	4.507769	5.942762	3.426052
C	5.283356	4.738194	3.424497
C	7.700028	3.222765	3.425279
C	9.122612	3.052805	3.426691
C	11.818235	3.979548	3.433640
C	12.831827	4.992866	3.435138
C	13.771116	7.683574	3.428773
C	13.614110	9.108781	3.423108
C	12.082519	11.513514	3.400210
C	7.009718	3.460209	4.644978
C	10.167600	12.480999	4.631824
C	8.744779	12.639980	4.639337
C	9.841617	3.128294	4.649512
C	11.194590	3.597928	4.652317
C	4.082387	8.044014	4.652712
C	4.256996	6.621959	4.649507
C	13.201630	5.621171	4.656102
C	13.667972	6.974847	4.654262
C	6.043341	11.736729	4.655912
C	5.020820	10.733789	4.657435
C	13.379241	9.810390	4.633921
C	12.649434	11.045650	4.616081
C	5.796346	4.221313	4.645158
C	10.871326	12.299326	5.842861
C	8.038321	12.562880	5.864884
C	6.681335	12.105091	5.872312
C	4.645151	10.113001	5.878801
C	4.166328	8.762742	5.876682
C	4.502735	5.933340	5.869284
C	5.274953	4.726770	5.867459
C	7.691259	3.212267	5.867154
C	9.113967	3.047055	5.868458
C	11.802182	3.991527	5.875528
C	12.805042	5.013074	5.877659
C	13.728893	7.710143	5.872532
C	13.591683	9.134656	5.867929
C	12.168666	11.631573	5.840180
C	7.001367	3.448042	7.087862
C	10.200896	12.549831	7.059188
C	8.777191	12.653947	7.077239

C	9.833037	3.124483	7.091202
C	11.182965	3.603393	7.093607
C	4.091781	8.036207	7.096138
C	4.256424	6.613479	7.093095
C	13.173027	5.642311	7.097510
C	13.635207	6.998276	7.096443
C	6.082379	11.713531	7.097162
C	5.055670	10.716783	7.099327
C	13.405923	9.847670	7.084787
C	12.772243	11.155921	7.069654
C	5.787852	4.209254	7.088448
C	10.955417	12.460129	8.288774
C	8.068238	12.566180	8.306570
C	6.722813	12.085129	8.313174
C	4.674972	10.099825	8.320444
C	4.183817	8.755534	8.319214
C	4.501051	5.925029	8.313338
C	5.269394	4.716382	8.311514
C	7.684788	3.202266	8.309864
C	9.107644	3.040634	8.310425
C	11.790385	3.999622	8.314968
C	12.786152	5.027132	8.316351
C	13.721245	7.730749	8.312722
C	13.634214	9.157477	8.300159
C	12.267957	11.756355	8.309685
C	6.997211	3.439316	9.532077
C	10.218948	12.624386	9.519151
C	8.798228	12.674175	9.525943
C	9.829040	3.121114	9.532589
C	11.176257	3.603835	9.533873
C	4.104139	8.031231	9.539177
C	4.259828	6.607995	9.536951
C	13.161020	5.653686	9.536648
C	13.629842	7.004478	9.537016
C	6.116373	11.696909	9.537437
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C	13.495323	9.884596	9.543473
C	12.750416	11.159942	9.553733
C	5.784210	4.200486	9.533045
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C	8.083719	12.568931	10.754581
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C	4.695729	10.094460	10.760448
C	4.199186	8.752690	10.760195
C	4.503614	5.921069	10.757710
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C	7.683033	3.195646	10.753686
C	9.106310	3.034863	10.753429
C	11.788853	3.995037	10.754111
C	12.784617	5.024123	10.755037
C	13.713201	7.718720	10.763755
C	13.597290	9.141566	10.773812
C	12.129243	11.583917	10.766920
C	6.998202	3.435254	11.976444
C	10.221722	12.666937	11.985461
C	8.798194	12.702566	11.981054
C	9.830178	3.114859	11.973880
C	11.179253	3.595365	11.973629

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C	4.266230	6.607657	11.979930
C	13.164447	5.637471	11.977191
C	13.620634	6.992763	11.980825
C	6.122076	11.703557	11.978481
C	5.097185	10.705817	11.978736
C	13.323710	9.821990	11.991385
C	12.615775	11.066308	11.984593
C	5.785525	4.197114	11.977832
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C	8.070815	12.607184	13.203102
C	6.730515	12.104028	13.198941
C	4.696432	10.099912	13.199218
C	4.205257	8.755215	13.200006
C	4.509845	5.922840	13.201407
C	5.273299	4.711189	13.200714
C	7.686343	3.193951	13.197570
C	9.109263	3.030989	13.196270
C	11.794670	3.982049	13.194862
C	12.792373	5.007487	13.196110
C	13.697010	7.710132	13.205901
C	13.537013	9.129630	13.212855
C	12.203112	11.694456	13.221524
C	7.003006	3.436138	14.420665
C	10.206665	12.625533	14.450830
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C	4.273459	6.611925	14.422000
C	13.178199	5.620700	14.417703
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C	5.083990	10.718408	14.417338
C	13.315054	9.820372	14.437597
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C	5.791100	4.199753	14.422075
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C	8.046163	12.615379	15.648401
C	6.699343	12.127637	15.641543
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C	4.517384	5.928856	15.643806
C	5.280613	4.716869	15.643913
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C	11.803816	3.970763	15.635855
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C	13.330442	9.800786	16.875599
C	12.582738	11.021709	16.882465
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C	8.024684	12.616369	18.090776
C	6.673466	12.141821	18.084027
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C	4.191663	8.768940	18.080002
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C	7.697780	3.200617	18.084264
C	9.120478	3.031249	18.082125
C	11.813466	3.964386	18.077678
C	12.821756	4.982579	18.077379
C	13.739767	7.682485	18.083206
C	13.574648	9.105287	18.089712
C	12.064974	11.524860	18.104790
C	7.016164	3.448712	19.306421
C	10.163120	12.522359	19.321081
C	8.740605	12.692426	19.315335
C	9.846961	3.109302	19.301556
C	11.201735	3.575778	19.299933
C	4.109326	8.048163	19.301975
C	4.280654	6.625724	19.303962
C	13.211523	5.596599	19.298197
C	13.673729	6.952807	19.300616
C	6.047660	11.758587	19.302306
C	5.035652	10.744425	19.299968
C	13.337804	9.785094	19.313425
C	12.573774	10.996654	19.319452
C	5.805946	4.215374	19.307080
C	10.843686	12.267788	20.540743
C	8.011884	12.610857	20.531744
C	6.656428	12.146357	20.526116
C	4.642004	10.130607	20.520480
C	4.179200	8.774392	20.521321
C	4.526408	5.943643	20.525873
C	5.294457	4.734264	20.527183
C	7.704460	3.208325	20.526569
C	9.126644	3.035448	20.524580
C	11.822802	3.959567	20.520120
C	12.834911	4.973526	20.519069
C	13.756492	7.671181	20.523636
C	13.583088	9.093186	20.528971
C	12.054170	11.502525	20.539739
C	7.022715	3.458175	21.748122
C	10.153140	12.505836	21.758372
C	8.731528	12.681212	21.754571
C	9.853125	3.111787	21.744289
C	11.209594	3.573467	21.742726
C	4.100842	8.052565	21.743097
C	4.279177	6.630929	21.744746
C	13.225732	5.586768	21.740448
C	13.688134	6.942729	21.741778

C	6.032630	11.762864	21.744868
C	5.018692	10.750691	21.742487
C	13.336862	9.773061	21.751482
C	12.566441	10.980497	21.756111
C	5.812203	4.224609	21.748141
C	10.835315	12.253575	22.977531
C	8.003287	12.604687	22.972025
C	6.645656	12.146787	22.968171
C	4.627862	10.135079	22.963246
C	4.168120	8.777997	22.963458
C	4.526522	5.949015	22.966466
C	5.298580	4.742191	22.967653
C	7.710243	3.217505	22.968254
C	9.132072	3.041200	22.966859
C	11.831391	3.955393	22.963083
C	12.846948	4.966018	22.961904
C	13.765736	7.662934	22.964325
C	13.585259	9.083966	22.968094
C	12.046146	11.487845	22.975637
C	7.027549	3.467890	24.189095
C	10.146156	12.494311	24.195674
C	8.724519	12.673231	24.193760
C	9.857839	3.116620	24.187137
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C	4.275597	6.634299	24.185859
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C	13.698330	6.935981	24.183801
C	6.021811	11.764968	24.187238
C	5.005965	10.754120	24.185539
C	13.335488	9.764189	24.189350
C	12.560424	10.968880	24.192478
C	5.816297	4.232865	24.188602
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C	4.616929	10.137477	25.406393
C	4.158772	8.779948	25.406171
C	4.524244	5.952386	25.407302
C	5.299863	4.747904	25.407930
C	7.713580	3.226147	25.409552
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C	12.040022	11.476506	25.411768
C	7.029104	3.474862	26.629618
C	10.139793	12.481235	26.633130
C	8.718923	12.664513	26.632832
C	9.859575	3.122729	26.629797
C	11.218602	3.576088	26.630152
C	4.085112	8.056439	26.627809
C	4.270954	6.635847	26.627439
C	13.245194	5.577461	26.627919
C	13.708605	6.933197	26.626866
C	6.013540	11.765018	26.630032
C	4.996802	10.755276	26.629270

C	13.339405	9.759863	26.626693
C	12.558185	10.960253	26.627787
C	5.816909	4.238044	26.628685
C	10.821907	12.224084	27.851192
C	7.992026	12.592674	27.851844
C	6.631053	12.144132	27.852140
C	4.609771	10.137786	27.850615
C	4.151809	8.779897	27.849872
C	4.519977	5.953041	27.848507
C	5.297555	4.749866	27.848357
C	7.713325	3.231331	27.850384
C	9.134926	3.054219	27.850828
C	11.837868	3.958885	27.852227
C	12.858495	4.964633	27.851875
C	13.785337	7.657652	27.847344
C	13.599332	9.077792	27.845247
C	12.036097	11.465219	27.846600
C	7.026139	3.476216	29.069604
C	10.134077	12.457872	29.070607
C	8.716081	12.651204	29.071065
C	9.857138	3.127479	29.072690
C	11.215769	3.582893	29.074050
C	4.079889	8.055230	29.071113
C	4.265639	6.634572	29.069575
C	13.244425	5.583379	29.073384
C	13.713918	6.937679	29.071532
C	6.010704	11.761850	29.073266
C	4.993023	10.753449	29.073858
C	13.351248	9.762601	29.063717
C	12.560098	10.955417	29.061593
C	5.813049	4.238041	29.068972
O	17.379159	15.605751	12.729469
O	13.439676	15.717600	13.323047
O	18.064234	16.232682	9.092121
O	12.945305	17.482626	9.701902
Pt	13.237658	16.629260	11.425800
Pt	15.542315	13.342583	8.096455
Pt	14.831554	15.331020	6.141428
Pt	16.364698	15.924620	8.176647
Pt	12.687586	13.817942	13.293861
Pt	14.937479	13.175755	11.903330
Pt	12.575925	13.916505	8.222665
Pt	13.621273	16.430128	8.163914
Pt	17.153554	15.765907	10.766479
Pt	15.004444	11.434267	9.816769
Pt	16.990062	13.101676	10.278700
Pt	15.428258	15.621921	12.830482
Pt	12.013023	14.306924	10.782378
Pt	14.526980	14.855997	10.005718
Pt	13.851449	12.927071	6.096088

Pt₁₅O₄@CNT: (in total 355 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma) 28.0000 28.0000 29.3063
90.0000 90.0000 90.0000

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C	9.377897	13.726310	0.985737
C	7.946312	13.694945	0.985695
C	5.510327	12.269428	0.986222
C	4.606195	11.141404	0.986530
C	3.836495	8.434152	0.983743
C	4.160044	7.038287	0.982317
C	5.919055	4.764871	0.976106
C	7.228984	4.160506	0.972714
C	10.105295	4.244300	0.986844
C	11.336549	4.979241	0.998428
C	13.096160	7.277677	0.996643
C	3.821034	9.161638	2.208552
C	13.512887	9.391672	2.209968
C	13.237607	10.807347	2.211021
C	4.458456	6.374873	2.205772
C	5.351722	5.245991	2.199677
C	7.238301	13.526931	2.209589
C	5.977083	12.828210	2.217253
C	7.973868	4.073606	2.199514
C	9.422821	4.053901	2.213177
C	11.419890	13.024213	2.206938
C	10.104219	13.609957	2.206030
C	11.926798	5.434885	2.208073
C	12.785166	6.598974	2.206864
C	4.167035	10.555479	2.216064
C	13.459852	8.653549	3.423724
C	12.899329	11.456918	3.430803
C	11.991334	12.574131	3.432256
C	9.389615	13.767239	3.426948
C	7.949675	13.711344	3.420609
C	5.354831	12.377286	3.411319
C	4.437511	11.253221	3.419405
C	3.829936	8.441683	3.431808
C	4.152802	7.039116	3.429778
C	5.942160	4.831888	3.436749
C	7.272810	4.247275	3.444779
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C	11.392577	4.941072	3.430297
C	13.107897	7.258777	3.422900
C	3.842847	9.188793	4.647283
C	13.470249	9.376926	4.647039
C	13.183401	10.780794	4.649365
C	4.471720	6.389349	4.654277
C	5.368963	5.272613	4.662762
C	7.251845	13.460918	4.642643
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C	10.098472	13.619816	4.653291
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C	12.865670	11.427449	5.875254
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C	9.374497	13.743947	5.874468
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C	9.407268	4.156536	7.098640
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C	9.349999	13.709856	8.314638
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C	4.177582	7.062279	8.315255
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C	5.986421	4.872140	13.199712
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C	5.357548	12.409103	18.082103
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C	7.290699	4.267475	18.076328
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C	7.199240	13.514587	19.303413
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C	11.977477	5.418870	19.304883
C	12.851376	6.554537	19.305645
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C	9.339791	13.716146	20.521862
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C	4.486866	11.268012	20.526064
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C	5.410509	5.309323	21.735213
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C	5.927957	12.859727	21.747719
C	7.991991	4.101122	21.736694
C	9.424265	4.130784	21.740321
C	11.354967	12.966306	21.739437
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C	11.964540	5.425942	21.749709
C	12.838221	6.561933	21.750425
C	4.183035	10.604056	21.746098
C	13.454491	8.624612	22.967213
C	12.832782	11.407815	22.959119
C	11.935280	12.524321	22.958876
C	9.347120	13.714624	22.964228
C	7.915183	13.680087	22.967045
C	5.373318	12.389108	22.969501
C	4.496589	11.256638	22.968968
C	3.877534	8.472689	22.962818
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C	7.927220	13.664143	25.408406
C	5.383792	12.375255	25.410841
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C	3.882173	8.460831	25.403546
C	4.194566	7.062843	25.401428
C	5.965353	4.832562	25.394829
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C	11.370840	4.978949	25.410863

C	13.119789	7.242276	25.412713
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C	13.454454	9.378976	26.623886
C	13.176885	10.785438	26.623769
C	4.507487	6.400725	26.619768
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C	11.900188	5.471185	26.632763
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C	4.504710	11.230912	27.852916
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C	5.957387	4.814499	27.838856
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C	3.848305	9.161054	29.065116
C	13.477054	9.389968	29.077030
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C	5.372898	5.249766	29.063384
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C	5.991597	12.810583	29.058303
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C	10.090125	13.569838	29.069295
C	11.779069	5.568718	29.077461
C	12.702981	6.673993	29.077245
C	4.202442	10.547408	29.058831
O	10.755525	9.872445	1.838344
O	8.607821	9.402587	-2.952928
O	7.312024	7.418268	7.497030
O	10.662385	9.185320	7.293833
Pt	7.054449	8.660494	5.935874
Pt	9.191269	7.933044	7.500745
Pt	10.131000	7.311920	-0.260237
Pt	10.375611	9.130854	-2.180733
Pt	6.900512	10.383995	1.108613
Pt	7.486854	9.623189	-1.363806
Pt	9.476571	10.026411	0.251121
Pt	7.227139	8.866201	3.316587
Pt	9.838847	7.973455	2.259838
Pt	9.369894	10.537448	3.149390
Pt	9.705143	10.038611	5.742545

Pt	7.606855	7.843194	0.545240
Pt	9.313113	7.591506	4.776435
Pt	7.459705	11.066343	4.877594
Pt	7.840944	6.394857	2.792314

Pt₁₅O₆/CNT: (in total 357 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
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C	4.149636	8.777146	0.988130
C	4.514265	5.949870	0.983792
C	5.291704	4.746679	0.982835
C	7.708562	3.230302	0.984356
C	9.130312	3.055919	0.985686
C	11.830997	3.968913	0.990179
C	12.850445	4.975750	0.990661
C	13.788776	7.665619	0.984053
C	13.611829	9.087288	0.979625
C	12.038139	11.460917	0.972978
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C	4.078466	8.051085	2.208770
C	4.260540	6.629734	2.206193
C	13.229662	5.599013	2.212747
C	13.702672	6.951609	2.210718
C	6.018436	11.753737	2.211751
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C	13.369303	9.780362	2.194903
C	12.583839	10.976982	2.188193
C	5.805691	4.232085	2.203450
C	10.848329	12.238791	3.408171
C	8.008077	12.572048	3.426029
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C	4.620695	10.125977	3.434836
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C	4.507769	5.942762	3.426052
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C	7.700028	3.222765	3.425279
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C	13.614110	9.108781	3.423108
C	12.082519	11.513514	3.400210
C	7.009718	3.460209	4.644978
C	10.167600	12.480999	4.631824
C	8.744779	12.639980	4.639337
C	9.841617	3.128294	4.649512
C	11.194590	3.597928	4.652317
C	4.082387	8.044014	4.652712
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C	8.038321	12.562880	5.864884
C	6.681335	12.105091	5.872312
C	4.645151	10.113001	5.878801
C	4.166328	8.762742	5.876682
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C	5.274953	4.726770	5.867459
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C	9.113967	3.047055	5.868458
C	11.802182	3.991527	5.875528
C	12.805042	5.013074	5.877659
C	13.728893	7.710143	5.872532
C	13.591683	9.134656	5.867929
C	12.168666	11.631573	5.840180
C	7.001367	3.448042	7.087862
C	10.200896	12.549831	7.059188
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C	5.055670	10.716783	7.099327
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C	12.772243	11.155921	7.069654
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C	4.183817	8.755534	8.319214
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C	11.176257	3.603835	9.533873
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C	4.259828	6.607995	9.536951
C	13.161020	5.653686	9.536648
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C	13.495323	9.884596	9.543473
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C	4.695729	10.094460	10.760448
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C	13.597290	9.141566	10.773812
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C	9.830178	3.114859	11.973880
C	11.179253	3.595365	11.973629
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C	4.266230	6.607657	11.979930
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C	12.834911	4.973526	20.519069
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C	5.812203	4.224609	21.748141
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C	8.003287	12.604687	22.972025
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C	7.710243	3.217505	22.968254
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C	12.846948	4.966018	22.961904
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C	6.013540	11.765018	26.630032
C	4.996802	10.755276	26.629270
C	13.339405	9.759863	26.626693
C	12.558185	10.960253	26.627787
C	5.816909	4.238044	26.628685
C	10.821907	12.224084	27.851192
C	7.992026	12.592674	27.851844
C	6.631053	12.144132	27.852140
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C	4.519977	5.953041	27.848507
C	5.297555	4.749866	27.848357
C	7.713325	3.231331	27.850384
C	9.134926	3.054219	27.850828
C	11.837868	3.958885	27.852227
C	12.858495	4.964633	27.851875
C	13.785337	7.657652	27.847344
C	13.599332	9.077792	27.845247
C	12.036097	11.465219	27.846600
C	7.026139	3.476216	29.069604
C	10.134077	12.457872	29.070607
C	8.716081	12.651204	29.071065
C	9.857138	3.127479	29.072690
C	11.215769	3.582893	29.074050
C	4.079889	8.055230	29.071113
C	4.265639	6.634572	29.069575
C	13.244425	5.583379	29.073384
C	13.713918	6.937679	29.071532
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C	12.560098	10.955417	29.061593
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O	17.372424	15.373821	12.856732
O	13.452865	15.705959	13.285107
O	18.136647	16.340325	9.260017

O	12.983506	17.466136	9.660998
O	14.510565	14.373418	4.811846
O	17.062647	13.512523	6.764643
Pt	13.341741	16.566369	11.332439
Pt	15.801211	13.129095	8.105992
Pt	15.298257	15.162992	6.421449
Pt	16.334642	16.366581	8.463093
Pt	12.691269	13.813030	13.304363
Pt	14.914142	13.121670	11.901928
Pt	12.664850	13.893727	8.209118
Pt	13.715949	16.416361	8.116555
Pt	17.314838	15.667646	10.899838
Pt	15.023934	11.392309	9.864923
Pt	17.070159	13.001791	10.439325
Pt	15.434205	15.537391	12.838578
Pt	12.173390	14.224365	10.765677
Pt	14.686449	14.752630	9.906909
Pt	13.847018	12.890525	6.009908

Pt₁₅O₆@CNT: (in total 357 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
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C	4.468786	11.315123	0.793866
C	3.863373	8.528523	0.791867
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C	5.980278	4.915597	0.788380
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C	10.127639	4.351547	0.790631
C	11.407382	4.995503	0.792753
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C	4.163745	10.653326	2.015080
C	13.444855	8.656861	3.236331
C	12.805676	11.436158	3.231268
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C	9.326492	13.756558	3.233489
C	7.893834	13.728442	3.235731
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C	4.473567	11.308424	3.237691

C	3.862793	8.522841	3.233024
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C	7.271451	4.298828	3.227010
C	10.121467	4.349571	3.233683
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C	13.443026	9.387585	4.455508
C	13.126376	10.785094	4.452317
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C	4.483290	11.297050	5.680595
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C	11.384074	5.005097	5.681075
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C	13.445773	9.399608	6.895635
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C	4.494188	6.441137	9.331395
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C	11.286113	5.073877	10.551568
C	13.069206	7.318053	10.558712
C	3.835006	9.201466	11.776743
C	13.463755	9.430380	11.788657
C	13.192964	10.838153	11.785947
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C	7.215685	4.200918	12.990646

C	10.091996	4.284712	13.004776
C	11.323250	5.019653	13.016360
C	13.082861	7.318089	13.014575
C	3.807735	9.202050	14.226484
C	13.499588	9.432084	14.227900
C	13.224308	10.847759	14.228953
C	4.445157	6.415285	14.223704
C	5.338423	5.286403	14.217609
C	7.225002	13.567343	14.227521
C	5.963784	12.868622	14.235185
C	7.960569	4.114018	14.217446
C	9.409522	4.094313	14.231109
C	11.406591	13.064625	14.224870
C	10.090920	13.650369	14.223962
C	11.913499	5.475297	14.226005
C	12.771867	6.639386	14.224796
C	4.153736	10.595891	14.233996
C	13.446553	8.693961	15.441656
C	12.886030	11.497330	15.448735
C	11.978035	12.614543	15.450188
C	9.376316	13.807651	15.444880
C	7.936376	13.751756	15.438541
C	5.341532	12.417698	15.429251
C	4.424212	11.293633	15.437337
C	3.816637	8.482095	15.449740
C	4.139503	7.079528	15.447710
C	5.928861	4.872300	15.454681
C	7.259511	4.287687	15.462711
C	10.121050	4.282123	15.454601
C	11.379278	4.981484	15.448229
C	13.094598	7.299189	15.440832
C	3.829548	9.229205	16.665215
C	13.456950	9.417338	16.664971
C	13.170102	10.821206	16.667297
C	4.458421	6.429761	16.672209
C	5.355664	5.313025	16.680694
C	7.238546	13.501330	16.660575
C	5.936148	12.843535	16.657005
C	7.971730	4.097768	16.691837
C	9.410543	4.120672	16.680382
C	11.387339	13.053020	16.670980
C	10.085173	13.660228	16.671223
C	11.921414	5.489872	16.664480
C	12.781873	6.640606	16.662265
C	4.108335	10.639694	16.662321
C	13.456632	8.686501	17.883491
C	12.852371	11.467861	17.893186
C	11.943257	12.579752	17.893907
C	9.361198	13.784359	17.892400
C	7.925497	13.718151	17.897949
C	5.351856	12.410747	17.895589
C	4.440688	11.293164	17.887294
C	3.867012	8.502613	17.890518
C	4.161968	7.095161	17.893669
C	5.938477	4.864460	17.897086
C	7.247548	4.266595	17.898669
C	10.105847	4.350002	17.897169
C	11.371874	5.027277	17.891117

C	13.113852	7.293917	17.880591
C	3.861432	9.230648	19.113880
C	13.491111	9.409469	19.106068
C	13.178502	10.810039	19.110470
C	4.464399	6.433846	19.114978
C	5.360634	5.311975	19.115131
C	7.199328	13.551599	19.111584
C	5.915843	12.896471	19.110829
C	7.962922	4.142269	19.119864
C	9.393969	4.196948	19.116572
C	11.361973	13.014846	19.117053
C	10.060882	13.617362	19.116494
C	11.932899	5.507070	19.104681
C	12.818845	6.632885	19.102218
C	4.158599	10.634555	19.111556
C	13.487117	8.675895	20.325185
C	12.845387	11.453855	20.332748
C	11.931264	12.557751	20.335416
C	9.336700	13.750268	20.332570
C	7.902032	13.725770	20.330661
C	5.353880	12.433711	20.328613
C	4.480933	11.295411	20.329084
C	3.861377	8.503992	20.333112
C	4.164283	7.102691	20.333187
C	5.940726	4.874782	20.337711
C	7.249590	4.291889	20.337983
C	10.099523	4.399708	20.332681
C	11.375920	5.047522	20.328121
C	13.151740	7.282225	20.322956
C	3.864709	9.237976	21.551388
C	13.480222	9.397401	21.549695
C	13.153614	10.793040	21.553058
C	4.483248	6.454688	21.556707
C	5.376599	5.334339	21.557020
C	7.192990	13.545551	21.550860
C	5.915133	12.898990	21.549926
C	7.969747	4.164614	21.555285
C	9.400526	4.216270	21.553389
C	11.345752	12.994877	21.554455
C	10.043823	13.592872	21.553487
C	11.946205	5.502753	21.545833
C	12.839029	6.623281	21.543626
C	4.176974	10.636762	21.550169
C	13.472125	8.666989	22.770048
C	12.822082	11.439050	22.774550
C	11.915893	12.548477	22.775804
C	9.329349	13.744296	22.772611
C	7.896762	13.720604	22.771634
C	5.352530	12.437360	22.769902
C	4.479134	11.301338	22.769950
C	3.862744	8.516787	22.774178
C	4.176859	7.118651	22.775065
C	5.959652	4.900246	22.778002
C	7.262922	4.307897	22.777427
C	10.112388	4.388833	22.770020
C	11.391394	5.032755	22.766829
C	13.157202	7.269860	22.768227
C	3.860483	9.248554	23.993261

C	13.461335	9.389279	23.994287
C	13.134300	10.783380	23.996174
C	4.495708	6.470104	23.998045
C	5.393566	5.354729	23.998588
C	7.188395	13.549243	23.991798
C	5.909223	12.905157	23.991163
C	7.981740	4.165032	23.994641
C	9.413532	4.200067	23.992070
C	11.338018	12.994626	23.995094
C	10.038221	13.597043	23.993767
C	11.962511	5.480198	23.988709
C	12.846255	6.607577	23.988693
C	4.168182	10.647534	23.992234
C	13.460261	8.659444	25.214306
C	12.808950	11.433960	25.216796
C	11.908447	12.548164	25.216664
C	9.324835	13.751341	25.213715
C	7.892363	13.727330	25.213547
C	5.345775	12.445992	25.212891
C	4.470970	11.311315	25.212962
C	3.861620	8.525621	25.216097
C	4.183287	7.129592	25.217157
C	5.973122	4.912552	25.217644
C	7.273252	4.311124	25.216219
C	10.124040	4.368141	25.210941
C	11.405066	5.010596	25.209580
C	13.155435	7.259593	25.212946
C	3.857777	9.255302	26.435655
C	13.449164	9.383731	26.436768
C	13.122716	10.778283	26.437553
C	4.504221	6.478469	26.437813
C	5.403992	5.364175	26.437516
C	7.184384	13.556611	26.434218
C	5.904240	12.912528	26.434110
C	7.988601	4.161772	26.434422
C	9.421011	4.187050	26.432676
C	11.333380	12.997015	26.435996
C	10.034971	13.603170	26.435062
C	11.969498	5.465006	26.432599
C	12.846589	6.597792	26.433526
C	4.162392	10.655210	26.435203
C	13.451731	8.654985	27.657346
C	12.801576	11.431292	27.657779
C	11.903989	12.547837	27.656955
C	9.322344	13.755845	27.655349
C	7.889659	13.732282	27.655819
C	5.342954	12.450857	27.656166
C	4.468067	11.316169	27.656436
C	3.862853	8.529494	27.657261
C	4.188358	7.134705	27.657447
C	5.980104	4.917453	27.656323
C	7.278036	4.311440	27.655217
C	10.128689	4.356535	27.653769
C	11.409296	4.999083	27.654201
C	13.151223	7.254378	27.657135
C	3.857991	9.256941	28.877944
C	13.442846	9.381062	28.878700
C	13.117451	10.776289	28.878141

C	4.508058	6.480802	28.876939
C	5.408017	5.366311	28.875870
C	7.183462	13.558511	28.877678
C	5.903488	12.914134	28.878111
C	7.990004	4.158056	28.874609
C	9.422722	4.179850	28.874626
C	11.331364	12.997964	28.876773
C	10.033615	13.605314	28.876521
C	11.969457	5.458838	28.877513
C	12.844090	6.593879	28.878475
C	4.161547	10.657094	28.878363
O	10.579495	9.991224	13.779688
O	8.247000	10.930957	8.996337
O	7.291704	7.500178	19.577110
O	10.639165	9.261333	19.276628
O	6.589871	8.196896	11.110741
O	10.390687	7.871680	9.762278
Pt	7.025126	8.661366	17.954950
Pt	9.171464	8.015615	19.544672
Pt	10.253132	7.499261	11.775579
Pt	9.614983	9.562503	9.389505
Pt	7.097840	10.523648	13.115342
Pt	7.249163	9.904011	10.403900
Pt	9.602404	10.092463	12.002115
Pt	7.194092	8.907899	15.341711
Pt	9.821849	8.054703	14.314404
Pt	9.228854	10.648640	15.137562
Pt	9.731081	10.065319	17.684385
Pt	7.741809	7.943445	12.652314
Pt	9.293142	7.581327	16.853025
Pt	7.419645	11.097109	16.986434
Pt	7.844027	6.422121	14.880088

The XYZ coordinates for the GSs of Pt₇₅/CNT, Pt₇₅@CNT, Pt₂₆₀/CNT and Pt₂₆₀@CNT

Pt ₇₅ /CNT(in total 75 atoms)			
Lattice Parameters (a, b, c, alpha, beta and gamma)			
90.0000	90.0000	90.0000	44.8948
Pt	6.896218719	18.099559626	19.200704875
Pt	11.500968776	16.781500936	21.654011395
Pt	9.010371925	19.825580422	16.515799035
Pt	8.805459130	22.095377801	12.513913454
Pt	8.853757514	22.084178410	17.829000911
Pt	3.353878215	16.875329226	13.839676615
Pt	4.612104103	18.827217355	15.152586471
Pt	7.757127628	15.543936995	19.255182166
Pt	5.083049317	11.806308514	16.433657401
Pt	8.634641397	13.010753167	11.042605140
Pt	8.835236716	22.155229155	15.170557612
Pt	11.619212388	16.782775594	16.441565976
Pt	4.160973689	14.324811692	16.468414505
Pt	9.267550303	17.430205102	15.145679875
Pt	5.474038382	16.196524990	17.918442871
Pt	3.360448723	16.890718520	16.477068439
Pt	12.733555155	14.698495320	17.781111991
Pt	8.623293522	12.982957484	19.188267888
Pt	6.399566968	13.647415593	15.130820163
Pt	6.742676701	20.438022972	17.847585652
Pt	11.275519503	19.173847945	12.498074906
Pt	5.101488992	11.802271327	13.794505940
Pt	11.597637203	16.810565353	19.101954194
Pt	11.600872810	16.800295670	13.771060020
Pt	11.297313167	19.203859230	15.150663998
Pt	6.350386829	13.644684811	12.355931437
Pt	8.661936968	12.984285225	16.489611879
Pt	4.675621629	18.718230989	12.509811586
Pt	11.190510076	19.103703362	20.429365764
Pt	8.994110748	19.831768563	13.800105932
Pt	9.198284282	17.478488813	12.397354351
Pt	10.090403690	14.886110474	17.864291667
Pt	5.517246583	16.221609155	15.152218940
Pt	11.290964771	19.175481578	17.802032435
Pt	7.282593678	11.164899898	12.467311052
Pt	9.887661506	11.092205811	17.799702308
Pt	6.889501726	18.131779018	13.791216229
Pt	9.190997724	17.438690836	9.770409387
Pt	7.256850797	11.160291454	17.762102166
Pt	10.953026970	21.413864935	11.226808611
Pt	7.779539825	15.554322575	16.547505911
Pt	11.122291080	19.155582771	9.922425014
Pt	11.004924540	21.393191655	19.094602620
Pt	10.131805894	14.872932711	15.143366654
Pt	4.702469263	18.732478357	17.795089227
Pt	9.202755402	17.421880234	20.555048905
Pt	11.408473442	12.819006093	16.471864376
Pt	6.339196389	13.641089149	17.897831046
Pt	10.031570185	14.895910194	20.538130096
Pt	11.281984223	12.899086083	19.155543731
Pt	12.599328986	14.775328125	20.391936999

Pt	6.699533829	20.442750801	12.489833033
Pt	6.867368972	18.103718064	11.098968277
Pt	9.220149018	17.455900960	17.896959487
Pt	8.877105070	19.844555800	11.051737073
Pt	9.913761207	11.124920326	12.414881309
Pt	12.753677865	14.715548617	15.103777409
Pt	6.714552189	20.516434010	15.168510280
Pt	7.752632494	15.558625699	11.009777315
Pt	6.905424434	18.127897485	16.513012055
Pt	11.049187769	21.547848802	13.828195597
Pt	10.052056797	14.915482910	12.436566935
Pt	11.485584647	16.808950041	11.074964557
Pt	8.937619220	19.819347372	19.262686844
Pt	4.167262509	14.316373496	13.808597094
Pt	5.463853351	16.192015018	12.376532643
Pt	9.932729163	11.040791186	15.110470773
Pt	11.069703546	21.545059329	16.486318502
Pt	8.660703873	12.985566910	13.760004744
Pt	7.761252454	15.561910138	13.740076313
Pt	7.269703204	11.030847089	15.117717418
Pt	12.660790982	14.766996833	12.444143552
Pt	10.066397617	14.952522604	9.825851177
Pt	11.418317102	12.836715825	13.763719452
Pt	11.266223985	12.979815866	11.111785076

Pt₇₅@CNT(in total 75 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	40.0000	40.0000	44.8948
90.0000 90.0000 90.0000			
Pt	19.686259730	24.461931822	23.959472583
Pt	16.203125806	21.164910304	16.171348205
Pt	18.475455573	17.444492895	22.893316310
Pt	19.996976064	21.677953528	18.722196271
Pt	21.862005707	23.644523136	25.304211175
Pt	20.529823287	18.655853474	21.454217773
Pt	24.775557265	20.232189579	17.390260814
Pt	23.846055668	22.393339358	21.315045028
Pt	19.736082281	24.436367922	26.567575843
Pt	21.636177781	17.146455822	25.625876503
Pt	16.267629660	21.238838599	21.458316249
Pt	21.805737155	23.500506636	22.637043393
Pt	20.473015535	18.549098211	18.822989830
Pt	22.178819904	20.880736539	25.412695158
Pt	16.224723762	21.199645862	18.806602851
Pt	23.326671203	18.541740845	16.020969717
Pt	17.895654782	22.623863422	14.738850336
Pt	18.296862992	17.379469186	14.874540016
Pt	20.052708689	21.890304793	26.829602440
Pt	20.540089224	19.001506471	24.106147197
Pt	21.575628222	22.998907271	14.617520538
Pt	18.217497391	17.257168379	17.531694061
Pt	16.349116230	18.568574977	16.242509019
Pt	19.620374644	24.167373228	15.953016720
Pt	23.204317186	18.890188901	26.838178665
Pt	18.327359821	20.031457908	20.145170411
Pt	16.347490728	21.274320442	24.101368958
Pt	20.047528356	21.763830428	21.401346644
Pt	21.723759880	23.279504379	17.254154327
Pt	18.337715767	17.351309860	20.206872262

Pt	20.006425441	15.818239285	18.818249185
Pt	20.296218541	18.654525502	16.181552792
Pt	17.891164195	22.858827083	20.051182879
Pt	18.231883520	19.964802781	17.473105189
Pt	19.991736675	15.786605607	24.184124914
Pt	24.828824154	20.377876777	22.758231138
Pt	17.969800118	22.931334837	25.381085871
Pt	20.555855872	19.237823208	26.822519223
Pt	20.119493767	18.787400383	13.557802792
Pt	18.371133220	20.137799384	22.819042332
Pt	22.133441129	20.574485665	20.050711277
Pt	20.020944467	15.807826355	21.515378246
Pt	19.925435533	15.840015748	16.138501584
Pt	16.357489993	18.602231881	18.916303906
Pt	16.444707224	18.646617569	21.599807292
Pt	23.794232605	22.296242811	18.609766084
Pt	23.343882760	18.667774014	24.203621496
Pt	23.379940939	18.490273791	18.755252564
Pt	19.681004096	24.390499317	21.291395249
Pt	19.861643961	21.419564267	13.418165564
Pt	21.958399208	20.334426420	14.652453217
Pt	21.787162201	23.554472726	27.894325125
Pt	18.367622319	20.244220181	25.531134121
Pt	21.766315453	23.391541536	19.955130296
Pt	19.929999400	21.501493635	16.042306162
Pt	18.803587684	17.637869199	25.545742863
Pt	22.059071702	16.691139767	20.161002758
Pt	22.228893648	20.988717002	28.054751115
Pt	24.807818048	20.312456438	20.058340182
Pt	21.968203922	16.835531074	22.915746711
Pt	16.631655801	18.695568581	24.259492335
Pt	20.056201521	21.859813328	24.104192751
Pt	17.892414934	22.937420743	22.723168636
Pt	23.840750477	22.530212511	26.699092075
Pt	18.060051626	19.974353487	14.727220573
Pt	22.191762413	20.718171760	22.718955586
Pt	19.659388138	24.323111339	18.616773957
Pt	23.627151868	22.022353736	15.909257393
Pt	23.893523029	22.492156990	24.011165167
Pt	17.844264008	22.815147282	17.377037790
Pt	21.688613269	17.039216298	14.696205045
Pt	22.070591264	20.460597470	17.381054825
Pt	22.006093041	16.724542093	17.373022934
Pt	24.794653832	20.461105436	25.433708362
Pt	23.369569972	18.578027818	21.475635427

Pt₂₆₀/CNT(in total 260 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	50.0000	50.0000	44.8948
90.0000	90.0000	90.0000	
Pt	36.272677673	39.019614473	18.125623742
Pt	39.734113163	33.436427980	25.603628896
Pt	38.031945399	34.943361354	19.878810089
Pt	33.666426749	33.581415487	16.858929097
Pt	34.005557456	35.902480533	15.349139812
Pt	31.663244111	37.772962127	17.833872559
Pt	40.017090644	38.147886878	25.370220891
Pt	33.305944945	41.321029328	28.861550669
Pt	33.492035276	41.152779794	26.086815769

Pt	31.218522519	42.928302292	28.474918774
Pt	39.417886795	33.642279266	28.282736756
Pt	29.173650183	42.247621428	24.331146497
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Pt	39.830819777	35.883021025	26.841186860
Pt	30.922355015	40.721481170	29.982761064
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Pt	37.317284450	32.922971507	26.848219601
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Pt	32.283529309	32.047667449	31.930911801
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Pt	30.386537841	33.572391020	29.066646855
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Pt	32.477165166	29.440613169	28.040472246
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Pt	30.335743225	36.141686545	32.842843297
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Pt	33.124956741	36.446692306	26.334452263
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Pt	28.533491028	35.206854537	26.020697686
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Pt	35.374806071	32.032635049	22.560199534
Pt	33.263687811	33.816604504	22.310783243
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Pt₂₆₀@CNT(in total 260 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)			50.0000	50.0000	44.8948
90.0000	90.0000	90.0000			
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Pt	22.689856177	23.055467539	27.383242979		
Pt	23.629173485	17.144541098	20.770333957		
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Pt	24.215196621	24.849602677	23.771832748
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Pt	24.099175418	24.909469597	31.074313682
Pt	13.537748328	16.616837444	22.206975792
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Pt	22.523884525	23.753930933	20.076629140
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Pt	20.791925731	12.269336198	33.173391546
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Pt	20.490209198	12.564352411	25.927717396
Pt	15.188898631	17.526409114	28.194055353
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Pt	26.627827632	17.218755864	34.396178646
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Pt	24.512462945	14.064310215	24.064187031
Pt	26.218884071	16.346131517	31.851393806

The XYZ coordinates for the C atoms in CNT(10, 10) and CNT(14, 14)

CNT(10, 10) (in total 720 atoms)
 Lattice Parameters (a, b, c, alpha, beta and gamma) 40.0000 40.0000 44.8948
 90.0000 90.0000 90.0000

C	26.969089037	22.076592529	0.246226498
C	26.411190832	23.403260055	0.246211739
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C	27.140995240	21.378365024	1.493277009
C	24.542212378	25.567261698	0.246225128
C	25.091448432	25.103373577	1.493314913
C	20.526798748	26.964742879	0.246244686
C	23.310896906	26.312537456	0.246224036
C	22.645171461	26.583981893	1.493300697
C	19.092574486	26.843940877	0.246214913
C	18.394451844	26.672249103	1.493292048
C	21.243817051	26.912289230	1.493314788
C	16.456847789	25.735135912	0.246254710
C	17.067765280	26.114145834	1.493318064
C	13.886924543	22.348102348	0.246229677
C	15.367560576	24.794373195	0.246220796
C	14.903659283	24.245134307	1.493302869
C	13.558652592	20.946743220	0.246235041
C	13.506195031	20.229723142	1.493306338
C	14.158401954	23.013806586	1.493321192
C	13.798688460	18.097388884	0.246216183
C	13.627026703	18.795510770	1.493295977
C	16.225806693	14.606595143	0.246212328
C	14.356786987	16.770697216	0.246241993
C	14.735796882	16.159774844	1.493307804
C	17.457129514	13.861322840	0.246214019
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C	15.676566842	15.070504598	1.493286186
C	20.241205454	13.209132530	0.246213719
C	19.524187009	13.261566105	1.493286465
C	24.311155282	14.438749716	0.246222943
C	21.675428834	13.329939430	0.246253500
C	22.373565146	13.501622555	1.493319409
C	25.400459333	15.379497668	0.246224920
C	25.864344678	15.928739912	1.493306237
C	23.700249171	14.059725520	1.493299915
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C	24.542212332	25.567261749	2.740378362
C	25.091448903	25.103373032	3.987467981
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C	23.310897000	26.312537428	2.740377235
C	22.645171450	26.583981899	3.987453720
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C	13.506195016	20.229723012	3.987459552
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C	26.969316167	22.076484734	32.670232805
C	26.411219471	23.403180910	32.670203389

C	26.032217694	24.014091202	33.917284253
C	27.140997673	21.378345413	33.917306448
C	24.542212332	25.567261749	32.670216362
C	25.091448903	25.103373032	33.917305981
C	20.526798654	26.964742896	32.670235884
C	23.310897000	26.312537428	32.670215235
C	22.645171450	26.583981899	33.917291720
C	19.092574576	26.843940909	32.670206112
C	18.394451831	26.672249100	33.917283072
C	21.243817064	26.912289230	33.917305812
C	16.456847703	25.735135870	32.670245909
C	17.067765291	26.114145842	33.917309087
C	13.886924498	22.348102261	32.670220868
C	15.367560630	24.794373274	32.670211995
C	14.903659274	24.245134298	33.917293892
C	13.558652589	20.946743301	32.670226801
C	13.506195016	20.229723012	33.917297552
C	14.158401958	23.013806597	33.917312214
C	13.798688484	18.097388765	32.670207377
C	13.627026702	18.795510753	33.917286998
C	16.225806760	14.606595074	32.670203529
C	14.356786995	16.770697194	32.670233002
C	14.735796874	16.159774858	33.917298827
C	17.457129422	13.861322868	32.670205220
C	18.122834583	13.589871945	33.917281887
C	15.676566829	15.070504610	33.917277210
C	20.241205463	13.209132530	32.670204730
C	19.524187025	13.261566104	33.917277486
C	24.311155183	14.438749668	32.670214144
C	21.675428856	13.329939436	32.670244511
C	22.373565041	13.501622539	33.917310612
C	25.400459396	15.379497759	32.670216119
C	25.864344613	15.928739848	33.917298002
C	23.700249239	14.059725574	33.917291679
C	26.881073574	17.825771848	32.670231750
C	26.609600291	17.160068850	33.917298745
C	27.209342066	19.227129355	32.670208423
C	27.261838720	19.944134241	33.917280482
C	26.969315958	22.076485688	35.164393725
C	26.411219409	23.403181058	35.164354898
C	26.032215391	24.014094838	36.411428607
C	27.140997469	21.378357358	36.411484916
C	24.542212331	25.567261750	35.164369296
C	25.091448449	25.103373562	36.411459025
C	20.526798653	26.964742896	35.164388886
C	23.310897001	26.312537427	35.164368237
C	22.645171449	26.583981899	36.411444720
C	19.092574577	26.843940909	35.164359114
C	18.394451831	26.672249100	36.411436072
C	21.243817064	26.912289230	36.411458812
C	16.456847702	25.735135870	35.164398911
C	17.067765291	26.114145842	36.411462087
C	13.886924498	22.348102265	35.164373870
C	15.367560631	24.794373275	35.164364997
C	14.903659274	24.245134298	36.411446893
C	13.558652590	20.946743330	35.164379803
C	13.506195002	20.229722896	36.411450362
C	14.158401958	23.013806596	36.411465216

C	13.798688496	18.097388736	35.164360377
C	13.627026704	18.795510726	36.411439994
C	16.225806761	14.606595073	35.164356529
C	14.356787060	16.770697098	35.164386194
C	14.735796881	16.159774845	36.411452388
C	17.457129421	13.861322868	35.164358220
C	18.122834581	13.589871945	36.411434878
C	15.676566830	15.070504608	36.411430201
C	20.241205373	13.209132546	35.164357911
C	19.524187012	13.261566104	36.411431041
C	24.311155277	14.438749714	35.164367878
C	21.675428926	13.329939463	35.164398254
C	22.373565231	13.501622565	36.411464167
C	25.400459337	15.379497673	35.164369855
C	25.864344762	15.928739995	36.411451002
C	23.700249075	14.059725449	36.411444671
C	26.881073585	17.825771882	35.164385301
C	26.609600243	17.160068680	36.411451740
C	27.209342065	19.227129414	35.164362105
C	27.261838430	19.944137192	36.411433871
C	26.969089023	22.076592624	37.658523698
C	26.411190891	23.403259978	37.658508940
C	26.032215362	24.014094888	38.905599026
C	27.140995243	21.378365012	38.905574033
C	24.542212311	25.567261767	37.658522329
C	25.091448443	25.103373569	38.905611936
C	20.526798653	26.964742896	37.658541886
C	23.310896998	26.312537429	37.658521237
C	22.645171449	26.583981899	38.905597721
C	19.092574577	26.843940909	37.658512114
C	18.394451831	26.672249100	38.905589072
C	21.243817064	26.912289230	38.905611812
C	16.456847702	25.735135870	37.658551911
C	17.067765291	26.114145842	38.905615087
C	13.886924498	22.348102263	37.658526878
C	15.367560631	24.794373275	37.658517997
C	14.903659274	24.245134298	38.905599893
C	13.558652590	20.946743316	37.658532242
C	13.506195029	20.229723129	38.905603362
C	14.158401958	23.013806598	38.905618216
C	13.798688474	18.097388788	37.658513384
C	13.627026699	18.795510783	38.905593000
C	16.225806760	14.606595074	37.658509529
C	14.356786928	16.770697292	37.658539194
C	14.735796888	16.159774833	38.905604827
C	17.457129422	13.861322868	37.658511220
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C	15.676566832	15.070504606	38.905583210
C	20.241205549	13.209132514	37.658510920
C	19.524186996	13.261566105	38.905583488
C	24.311155368	14.438749759	37.658520144
C	21.675428743	13.329939398	37.658550701
C	22.373565158	13.501622557	38.905616433
C	25.400459278	15.379497588	37.658522121
C	25.864344687	15.928739921	38.905603261
C	23.700249160	14.059725513	38.905596938
C	26.881073585	17.825771868	37.658537748
C	26.609600267	17.160068764	38.905604564

C	27.209342075	19.227129407	37.658515072
C	27.261838263	19.944139087	38.905586784
C	26.969316167	22.076484735	40.152691807
C	26.411219472	23.403180909	40.152662391
C	26.032217695	24.014091201	41.399743255
C	27.140997673	21.378345413	41.399765449
C	24.542212331	25.567261750	40.152675364
C	25.091448902	25.103373032	41.399764983
C	20.526798653	26.964742896	40.152694886
C	23.310897001	26.312537427	40.152674237
C	22.645171450	26.583981898	41.399750722
C	19.092574577	26.843940909	40.152665114
C	18.394451832	26.672249101	41.399742074
C	21.243817063	26.912289230	41.399764814
C	16.456847702	25.735135870	40.152704911
C	17.067765290	26.114145841	41.399768089
C	13.886924497	22.348102260	40.152679870
C	15.367560631	24.794373275	40.152670997
C	14.903659275	24.245134299	41.399752894
C	13.558652589	20.946743302	40.152685803
C	13.506195016	20.229723013	41.399756554
C	14.158401958	23.013806596	41.399771216
C	13.798688484	18.097388764	40.152666379
C	13.627026702	18.795510752	41.399746000
C	16.225806761	14.606595074	40.152662531
C	14.356786994	16.770697195	40.152692004
C	14.735796873	16.159774858	41.399757829
C	17.457129421	13.861322868	40.152664222
C	18.122834582	13.589871945	41.399740889
C	15.676566829	15.070504609	41.399736212
C	20.241205464	13.209132530	40.152663732
C	19.524187026	13.261566104	41.399736488
C	24.311155184	14.438749668	40.152673146
C	21.675428855	13.329939436	40.152703513
C	22.373565041	13.501622539	41.399769614
C	25.400459395	15.379497758	40.152675121
C	25.864344612	15.928739848	41.399757004
C	23.700249240	14.059725575	41.399750681
C	26.881073575	17.825771849	40.152690752
C	26.609600291	17.160068851	41.399757746
C	27.209342066	19.227129354	40.152667425
C	27.261838720	19.944134240	41.399739484
C	26.969315960	22.076485675	42.646852749
C	26.411219401	23.403181069	42.646813922
C	26.032215434	24.014094752	43.893887807
C	27.140997437	21.378357449	43.893944117
C	24.542212340	25.567261741	42.646828320
C	25.091448369	25.103373617	43.893918225
C	20.526798666	26.964742894	42.646847910
C	23.310896988	26.312537431	42.646827261
C	22.645171535	26.583981854	43.893903921
C	19.092574565	26.843940905	42.646818137
C	18.394451927	26.672249114	43.893895273
C	21.243816967	26.912289227	43.893918012
C	16.456847714	25.735135876	42.646857934
C	17.067765215	26.114145783	43.893921288
C	13.886924504	22.348102277	42.646832893
C	15.367560623	24.794373264	42.646824021

C	14.903659343	24.245134365	43.893906093
C	13.558652590	20.946743317	42.646838826
C	13.506195019	20.229722991	43.893909563
C	14.158401930	23.013806504	43.893924417
C	13.798688493	18.097388749	42.646819401
C	13.627026736	18.795510635	43.893899195
C	16.225806752	14.606595082	42.646815553
C	14.356787068	16.770697088	42.646845217
C	14.735796838	16.159774932	43.893911589
C	17.457129433	13.861322864	42.646817244
C	18.122834496	13.589871990	43.893894079
C	15.676566910	15.070504553	43.893889402
C	20.241205360	13.209132547	42.646816935
C	19.524187108	13.261566107	43.893890242
C	24.311155266	14.438749708	42.646826902
C	21.675428939	13.329939466	42.646857277
C	22.373565135	13.501622552	43.893923368
C	25.400459345	15.379497684	42.646828879
C	25.864344693	15.928739927	43.893910203
C	23.700249151	14.059725507	43.893903871
C	26.881073579	17.825771871	42.646844324
C	26.609600270	17.160068772	43.893910941
C	27.209342065	19.227129427	42.646821128
C	27.261838414	19.944137097	43.893893072

CNT(14, 14) (in total 1008 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)			50.0000	50.0000	44.8948
90.0000	90.0000	90.0000			
C	29.359232255	19.977508342	0.335760113		
C	28.179187172	24.096062567	0.335760113		
C	29.173441873	21.404590135	0.335760113		
C	29.001234103	22.103264805	1.582836894		
C	27.392607731	25.301207925	0.335760113		
C	26.934311128	25.855974425	1.582836894		
C	28.502547021	23.453224588	1.582836894		
C	25.329028932	27.294750337	0.335760113		
C	25.899283014	26.855874120	1.582836894		
C	21.373266729	28.940031641	0.335760113		
C	24.097452898	28.039265172	0.335760113		
C	23.443837509	28.340244749	1.582836894		
C	19.940622236	29.076454974	0.335760113		
C	19.221144683	29.064034239	1.582836894		
C	22.077469585	28.792041527	1.582836894		
C	17.095388006	28.706037037	0.335760113		
C	17.794062832	28.878244873	1.582836894		
C	13.342678685	26.639113217	0.335760113		
C	15.745427608	28.207349089	0.335760113		
C	15.102589618	27.883989290	1.582836894		
C	12.342778805	25.604085945	0.335760113		
C	11.903902659	25.033831926	1.582836894		
C	13.897444856	27.097410597	1.582836894		
C	10.858408284	23.148639567	0.335760113		
C	11.159387796	23.802255837	1.582836894		
C	10.134618761	18.925947673	0.335760113		
C	10.406611491	21.782271662	0.335760113		
C	10.258621343	21.078069665	1.582836894		
C	10.320408144	17.498865775	0.335760113		

C	10.492615893	16.800190210	1.582836894
C	10.122198025	19.645425226	1.582836894
C	11.314663787	14.807392505	0.335760113
C	10.991303964	15.450230472	1.582836894
C	14.164820970	11.608704710	0.335760113
C	12.101242326	13.602246968	0.335760113
C	12.559539700	13.047480760	1.582836894
C	15.396397226	10.864190762	0.335760113
C	16.050013432	10.563211285	1.582836894
C	13.594567175	12.047581716	1.582836894
C	18.120583338	9.963424342	0.335760113
C	17.416381342	10.111414490	1.582836894
C	22.398462742	10.197418880	0.335760113
C	19.553227769	9.827001038	0.335760113
C	20.272705345	9.839420746	1.582836894
C	23.748422576	10.696105974	0.335760113
C	24.391260494	11.019465786	1.582836894
C	21.699787206	10.025211148	1.582836894
C	26.151172322	12.264341779	0.335760113
C	25.596406038	11.806044331	1.582836894
C	28.635441752	15.754815498	0.335760113
C	27.151071202	13.299370097	0.335760113
C	27.589948282	13.869623958	1.582836894
C	29.087238527	17.121183411	0.335760113
C	29.235228639	17.825386267	1.582836894
C	28.334462208	15.101200172	1.582836894
C	29.371651962	19.258030767	1.582836894
C	29.359232255	19.977508335	2.829913111
C	28.179187175	24.096062560	2.829913111
C	29.173441871	21.404590142	2.829913111
C	29.001234115	22.103264748	4.076990000
C	27.392607726	25.301207930	2.829913111
C	26.934311164	25.855974379	4.076990000
C	28.502546993	23.453224641	4.076990000
C	25.329028937	27.294750333	2.829913111
C	25.899282967	26.855874154	4.076990000
C	21.373266735	28.940031638	2.829913111
C	24.097452891	28.039265175	2.829913111
C	23.443837561	28.340244723	4.076990000
C	19.940622229	29.076454974	2.829913111
C	19.221144742	29.064034240	4.076990000
C	22.077469528	28.792041538	4.076990000
C	17.095388013	28.706037038	2.829913111
C	17.794062776	28.878244858	4.076990000
C	13.342678691	26.639113222	2.829913111
C	15.745427602	28.207349086	2.829913111
C	15.102589671	27.883989316	4.076990000
C	12.342778802	25.604085939	2.829913111
C	11.903902696	25.033831972	4.076990000
C	13.897444812	27.097410559	4.076990000
C	10.858408287	23.148639574	2.829913111
C	11.159387772	23.802255784	4.076990000
C	10.134618761	18.925947681	2.829913111
C	10.406611490	21.782271655	2.829913111
C	10.258621357	21.078069722	4.076990000
C	10.320408146	17.498865769	2.829913111
C	10.492615880	16.800190267	4.076990000
C	10.122198028	19.645425168	4.076990000

C	11.314663784	14.807392511	2.829913111
C	10.991303991	15.450230420	4.076990000
C	14.164820964	11.608704714	2.829913111
C	12.101242330	13.602246963	2.829913111
C	12.559539663	13.047480806	4.076990000
C	15.396397232	10.864190759	2.829913111
C	16.050013379	10.563211310	4.076990000
C	13.594567223	12.047581682	4.076990000
C	18.120583332	9.963424344	2.829913111
C	17.416381399	10.111414479	4.076990000
C	22.398462735	10.197418878	2.829913111
C	19.553227777	9.827001038	2.829913111
C	20.272705286	9.839420746	4.076990000
C	23.748422582	10.696105977	2.829913111
C	24.391260440	11.019465762	4.076990000
C	21.699787262	10.025211163	4.076990000
C	26.151172316	12.264341774	2.829913111
C	25.596406082	11.806044370	4.076990000
C	28.635441749	15.754815492	2.829913111
C	27.151071206	13.299370102	2.829913111
C	27.589948245	13.869623912	4.076990000
C	29.087238529	17.121183419	2.829913111
C	29.235228626	17.825386210	4.076990000
C	28.334462232	15.101200226	4.076990000
C	29.371651960	19.258030826	4.076990000
C	29.359232255	19.977508335	5.324066889
C	28.179187175	24.096062560	5.324066889
C	29.173441871	21.404590142	5.324066889
C	29.001234103	22.103264805	6.571143106
C	27.392607726	25.301207930	5.324066889
C	26.934311128	25.855974425	6.571143106
C	28.502547021	23.453224589	6.571143106
C	25.329028937	27.294750333	5.324066889
C	25.899283014	26.855874120	6.571143106
C	21.373266735	28.940031638	5.324066889
C	24.097452891	28.039265175	5.324066889
C	23.443837509	28.340244749	6.571143106
C	19.940622229	29.076454974	5.324066889
C	19.221144683	29.064034239	6.571143106
C	22.077469585	28.792041527	6.571143106
C	17.095388013	28.706037038	5.324066889
C	17.794062832	28.878244873	6.571143106
C	13.342678691	26.639113222	5.324066889
C	15.745427602	28.207349086	5.324066889
C	15.102589619	27.883989290	6.571143106
C	12.342778802	25.604085939	5.324066889
C	11.903902659	25.033831927	6.571143106
C	13.897444856	27.097410597	6.571143106
C	10.858408287	23.148639574	5.324066889
C	11.159387796	23.802255837	6.571143106
C	10.134618761	18.925947681	5.324066889
C	10.406611490	21.782271655	5.324066889
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C	25.596406038	11.806044331	36.500981106
C	28.635441749	15.754815492	35.253904889
C	27.151071206	13.299370102	35.253904889
C	27.589948282	13.869623958	36.500981106
C	29.087238529	17.121183419	35.253904889
C	29.235228639	17.825386267	36.500981106
C	28.334462208	15.101200173	36.500981106
C	29.371651962	19.258030767	36.500981106
C	29.359232255	19.977508338	37.748057894

C	28.179187174	24.096062563	37.748057894
C	29.173441871	21.404590139	37.748057894
C	29.001234103	22.103264805	38.995134106
C	27.392607729	25.301207929	37.748057894
C	26.934311128	25.855974425	38.995134106
C	28.502547021	23.453224589	38.995134106
C	25.329028935	27.294750335	37.748057894
C	25.899283014	26.855874120	38.995134106
C	21.373266733	28.940031639	37.748057894
C	24.097452894	28.039265174	37.748057894
C	23.443837509	28.340244749	38.995134106
C	19.940622232	29.076454974	37.748057894
C	19.221144683	29.064034239	38.995134106
C	22.077469585	28.792041527	38.995134106
C	17.095388010	28.706037037	37.748057894
C	17.794062832	28.878244873	38.995134106
C	13.342678689	26.639113220	37.748057894
C	15.745427604	28.207349087	37.748057894
C	15.102589619	27.883989290	38.995134106
C	12.342778803	25.604085941	37.748057894
C	11.903902659	25.033831926	38.995134106
C	13.897444856	27.097410597	38.995134106
C	10.858408286	23.148639571	37.748057894
C	11.159387796	23.802255837	38.995134106
C	10.134618761	18.925947677	37.748057894
C	10.406611490	21.782271658	37.748057894
C	10.258621343	21.078069665	38.995134106
C	10.320408145	17.498865771	37.748057894
C	10.492615893	16.800190210	38.995134106
C	10.122198025	19.645425226	38.995134106
C	11.314663785	14.807392508	37.748057894
C	10.991303964	15.450230471	38.995134106
C	14.164820966	11.608704712	37.748057894
C	12.101242329	13.602246965	37.748057894
C	12.559539700	13.047480760	38.995134106
C	15.396397230	10.864190761	37.748057894
C	16.050013432	10.563211285	38.995134106
C	13.594567175	12.047581716	38.995134106
C	18.120583335	9.963424343	37.748057894
C	17.416381342	10.111414490	38.995134106
C	22.398462738	10.197418878	37.748057894
C	19.553227774	9.827001038	37.748057894
C	20.272705345	9.839420746	38.995134106
C	23.748422580	10.696105976	37.748057894
C	24.391260493	11.019465786	38.995134106
C	21.699787206	10.025211148	38.995134106
C	26.151172319	12.264341775	37.748057894
C	25.596406038	11.806044331	38.995134106
C	28.635441751	15.754815494	37.748057894
C	27.151071204	13.299370100	37.748057894
C	27.589948282	13.869623958	38.995134106
C	29.087238527	17.121183415	37.748057894
C	29.235228639	17.825386267	38.995134106
C	28.334462208	15.101200172	38.995134106
C	29.371651962	19.258030767	38.995134106
C	29.359232255	19.977508338	40.242210894
C	28.179187174	24.096062563	40.242210894
C	29.173441871	21.404590139	40.242210894

C	29.001234104	22.103264802	41.489287111
C	27.392607729	25.301207929	40.242210894
C	26.934311130	25.855974423	41.489287111
C	28.502547019	23.453224592	41.489287111
C	25.329028935	27.294750335	40.242210894
C	25.899283012	26.855874121	41.489287111
C	21.373266733	28.940031639	40.242210894
C	24.097452894	28.039265174	40.242210894
C	23.443837512	28.340244748	41.489287111
C	19.940622232	29.076454974	40.242210894
C	19.221144687	29.064034239	41.489287111
C	22.077469582	28.792041529	41.489287111
C	17.095388011	28.706037037	40.242210894
C	17.794062830	28.878244873	41.489287111
C	13.342678689	26.639113220	40.242210894
C	15.745427604	28.207349087	40.242210894
C	15.102589621	27.883989291	41.489287111
C	12.342778803	25.604085941	40.242210894
C	11.903902662	25.033831929	41.489287111
C	13.897444854	27.097410595	41.489287111
C	10.858408286	23.148639571	40.242210894
C	11.159387795	23.802255835	41.489287111
C	10.134618761	18.925947677	40.242210894
C	10.406611490	21.782271658	40.242210894
C	10.258621344	21.078069668	41.489287111
C	10.320408145	17.498865771	40.242210894
C	10.492615891	16.800190212	41.489287111
C	10.122198025	19.645425223	41.489287111
C	11.314663785	14.807392508	40.242210894
C	10.991303965	15.450230469	41.489287111
C	14.164820966	11.608704712	40.242210894
C	12.101242329	13.602246965	40.242210894
C	12.559539697	13.047480762	41.489287111
C	15.396397230	10.864190761	40.242210894
C	16.050013429	10.563211286	41.489287111
C	13.594567178	12.047581715	41.489287111
C	18.120583335	9.963424343	40.242210894
C	17.416381345	10.111414490	41.489287111
C	22.398462738	10.197418878	40.242210894
C	19.553227774	9.827001038	40.242210894
C	20.272705341	9.839420746	41.489287111
C	23.748422580	10.696105976	40.242210894
C	24.391260490	11.019465785	41.489287111
C	21.699787209	10.025211149	41.489287111
C	26.151172319	12.264341775	40.242210894
C	25.596406041	11.806044334	41.489287111
C	28.635441751	15.754815494	40.242210894
C	27.151071204	13.299370100	40.242210894
C	27.589948281	13.869623955	41.489287111
C	29.087238527	17.121183415	40.242210894
C	29.235228639	17.825386264	41.489287111
C	28.334462209	15.101200176	41.489287111
C	29.371651962	19.258030771	41.489287111
C	29.359232255	19.977508280	42.736364000
C	28.179187199	24.096062510	42.736364000
C	29.173441856	21.404590196	42.736364000
C	29.001234102	22.103264806	43.983440882
C	27.392607690	25.301207973	42.736364000

C	26.934311127	25.855974426	43.983440882
C	28.502547021	23.453224588	43.983440882
C	25.329028980	27.294750298	42.736364000
C	25.899283015	26.855874119	43.983440881
C	21.373266790	28.940031626	42.736364000
C	24.097452841	28.039265196	42.736364000
C	23.443837508	28.340244750	43.983440881
C	19.940622174	29.076454972	42.736364000
C	19.221144682	29.064034239	43.983440881
C	22.077469586	28.792041527	43.983440881
C	17.095388067	28.706037050	42.736364000
C	17.794062834	28.878244874	43.983440881
C	13.342678734	26.639113256	42.736364000
C	15.745427553	28.207349060	42.736364000
C	15.102589618	27.883989289	43.983440881
C	12.342778769	25.604085894	42.736364000
C	11.903902658	25.033831925	43.983440881
C	13.897444857	27.097410597	43.983440881
C	10.858408311	23.148639624	42.736364000
C	11.159387795	23.802255838	43.983440882
C	10.134618762	18.925947735	42.736364000
C	10.406611479	21.782271602	42.736364000
C	10.258621343	21.078069664	43.983440881
C	10.320408160	17.498865716	42.736364000
C	10.492615892	16.800190209	43.983440881
C	10.122198025	19.645425227	43.983440881
C	11.314663761	14.807392561	42.736364000
C	10.991303963	15.450230473	43.983440881
C	14.164820921	11.608704748	42.736364000
C	12.101242367	13.602246922	42.736364000
C	12.559539700	13.047480759	43.983440881
C	15.396397283	10.864190738	42.736364000
C	16.050013433	10.563211284	43.983440881
C	13.594567175	12.047581717	43.983440881
C	18.120583278	9.963424357	42.736364000
C	17.416381340	10.111414490	43.983440881
C	22.398462681	10.197418866	42.736364000
C	19.553227832	9.827001039	42.736364000
C	20.272705346	9.839420746	43.983440882
C	23.748422631	10.696106003	42.736364000
C	24.391260494	11.019465787	43.983440881
C	21.699787205	10.025211148	43.983440881
C	26.151172274	12.264341739	42.736364000
C	25.596406037	11.806044331	43.983440881
C	28.635441724	15.754815442	42.736364000
C	27.151071238	13.299370147	42.736364000
C	27.589948283	13.869623959	43.983440881
C	29.087238538	17.121183472	42.736364000
C	29.235228640	17.825386268	43.983440881
C	28.334462207	15.101200172	43.983440881
C	29.371651962	19.258030766	43.983440882

The XYZ coordinates for the ISs and TSs of O-O dissociation on Pt₁₅, Pt₁₅O₂, Pt₁₅O₄ and Pt₁₅O₆ (the C atoms are not listed for simplicity)

IS on Pt₁₅/CNT: (in total 17 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	16.128250	10.682826	11.531101
O	17.509393	11.004435	11.460664
Pt	15.092715	11.947292	4.475982
Pt	17.481949	12.873416	7.692821
Pt	15.745115	9.146556	4.477445
Pt	18.293280	9.358356	7.693966
Pt	15.744686	9.146178	7.262376
Pt	16.047193	14.148812	5.887608
Pt	15.096429	11.948821	7.262344
Pt	17.454897	12.893708	4.099868
Pt	17.645171	11.059495	5.897371
Pt	18.282988	9.327453	4.100951
Pt	15.521793	10.572094	9.530401
Pt	17.565125	7.583889	5.890560
Pt	18.015104	11.146071	9.518074
Pt	15.516462	10.567602	2.198416
Pt	18.032721	11.148159	2.302093

IS on Pt₁₅@CNT: (in total 17 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	8.844054	7.716590	15.204896
O	7.808430	8.731078	15.144866
Pt	9.917300	7.844923	13.501406
Pt	10.703103	10.414047	13.276572
Pt	8.109466	7.348895	6.821131
Pt	8.852533	9.955110	6.445409
Pt	6.495320	9.813363	11.162939
Pt	7.841015	10.086511	8.866394
Pt	10.720926	8.083793	6.723586
Pt	6.694489	7.667520	9.245848
Pt	10.586710	10.269722	8.620914
Pt	8.053059	9.701604	13.384866
Pt	9.129148	10.552596	11.087461
Pt	6.240799	9.229733	6.916088
Pt	10.909631	8.608277	11.113319
Pt	8.254595	7.732717	11.390446
Pt	9.489383	7.797335	9.051138

TS on Pt₁₅/CNT: (in total 17 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	15.977870	10.639117	11.429018
O	18.057322	11.142987	11.170804
Pt	15.091529	11.943876	4.452260
Pt	17.474073	12.970546	7.667790
Pt	15.742348	9.148106	4.450517
Pt	18.331216	9.269157	7.664903
Pt	15.753086	9.169787	7.244760

Pt	16.024752	14.147896	5.853498
Pt	15.113242	11.929245	7.249959
Pt	17.454899	12.888231	4.082643
Pt	17.636603	11.059377	5.900905
Pt	18.280710	9.335898	4.084480
Pt	15.605200	10.583284	9.548782
Pt	17.545192	7.574051	5.852634
Pt	18.078412	11.159675	9.346623
Pt	15.517756	10.568979	2.177702
Pt	18.035790	11.150199	2.277627

TS on Pt₁₅@CNT: (in total 17 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
<i>O</i>	8.989985	7.660044	15.199084
<i>O</i>	7.695550	8.989213	15.116974
Pt	9.870836	7.871497	13.536957
Pt	10.699747	10.410851	13.280255
Pt	8.119264	7.357168	6.816094
Pt	8.856990	9.961343	6.424941
Pt	6.519539	9.802905	11.148674
Pt	7.851281	10.090564	8.849797
Pt	10.728718	8.100032	6.691906
Pt	6.706058	7.669015	9.237041
Pt	10.589055	10.281853	8.602045
Pt	7.996072	9.695522	13.386866
Pt	9.140830	10.534028	11.086000
Pt	6.241887	9.231422	6.913848
Pt	10.909139	8.578752	11.128749
Pt	8.280529	7.717969	11.377061
Pt	9.509204	7.803551	9.030364

IS on Pt₁₅O₂/CNT: (in total 19 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
<i>O</i>	19.656225	8.863862	3.091198
<i>O</i>	19.464565	9.961699	2.175488
<i>O</i>	18.817720	9.453555	9.126040
<i>O</i>	17.905738	13.152282	9.152810
Pt	15.094303	11.936575	4.497209
Pt	17.196189	13.518456	7.377180
Pt	15.750257	9.191257	4.546555
Pt	18.349316	8.759489	7.369191
Pt	15.733510	8.989247	7.386798
Pt	15.334473	14.252149	5.735690
Pt	14.993499	12.098213	7.383417
Pt	17.443998	13.049173	4.548797
Pt	17.305558	11.020868	6.239381
Pt	18.359104	9.275658	4.601033
Pt	15.520757	10.584648	9.517264
Pt	17.033479	7.204714	5.756933
Pt	18.059602	11.226490	9.145622
Pt	15.540389	10.600596	2.251083
Pt	18.034777	11.161507	2.874807

IS on Pt₁₅O₂@CNT: (in total 19 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	10.409821	9.066675	4.522916
O	9.450949	10.110911	4.572738
O	9.064121	7.807727	14.890918
O	6.797711	10.115320	13.330738
Pt	10.320470	7.497215	13.320223
Pt	10.789716	10.329144	13.264521
Pt	8.042063	7.397046	6.783123
Pt	8.665691	10.174646	6.429177
Pt	6.642065	9.458799	11.394292
Pt	7.854781	10.080380	8.931538
Pt	10.557474	8.369740	6.470033
Pt	6.804786	7.671551	9.293691
Pt	10.532967	10.330779	8.599449
Pt	8.435333	9.192667	13.614240
Pt	9.244644	10.302893	11.103509
Pt	6.192557	9.246028	6.979557
Pt	11.128952	8.506940	10.939472
Pt	8.513918	7.462347	11.323774
Pt	9.592471	7.816580	8.880040

TS on Pt₁₅O₂/CNT: (in total 19 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	19.399380	10.254398	2.101188
O	19.726254	8.777280	3.355572
O	18.807793	9.451395	9.120426
O	17.900784	13.151620	9.155744
Pt	15.107500	11.926684	4.504662
Pt	17.205735	13.491648	7.369175
Pt	15.751245	9.173360	4.539840
Pt	18.341002	8.752140	7.364973
Pt	15.725997	8.963287	7.407881
Pt	15.353658	14.254756	5.725476
Pt	14.975808	12.115264	7.397103
Pt	17.469315	13.063897	4.572404
Pt	17.256124	10.982262	6.230472
Pt	18.387494	9.215788	4.585865
Pt	15.518868	10.588191	9.514706
Pt	17.009719	7.188097	5.771244
Pt	18.054263	11.226388	9.146199
Pt	15.526505	10.596221	2.245496
Pt	17.999368	11.139412	2.918529

TS on Pt₁₅O₂@CNT: (in total 19 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	8.539398	9.567196	4.666594
O	8.139576	7.756567	4.813168
O	9.024124	7.738586	14.869844
O	6.747902	10.029024	13.296828
Pt	10.352139	7.515653	13.346078
Pt	10.785567	10.316075	13.281274
Pt	8.128424	7.508955	6.696075

Pt	8.972491	10.049786	6.436807
Pt	6.670042	9.515244	11.318243
Pt	7.869269	10.141033	8.920020
Pt	10.859647	8.164553	6.708723
Pt	6.860721	7.644104	9.220380
Pt	10.538298	10.285232	8.628719
Pt	8.409195	9.158268	13.623296
Pt	9.261658	10.307234	11.124151
Pt	6.206204	9.292462	7.019438
Pt	11.161898	8.514091	10.956445
Pt	8.506499	7.493612	11.350883
Pt	9.536216	7.753166	8.954348

IS on Pt₁₅O₄/CNT: (in total 21 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)			28.0000	28.0000	29.3063
90.0000	90.0000	90.0000			
O	14.646416	14.996277	4.225969		
O	14.023575	13.708355	4.112769		
O	17.331172	15.490237	12.788631		
O	13.419655	15.738348	13.346065		
O	18.057685	16.127516	9.079320		
O	12.895679	17.485943	9.728173		
Pt	13.194406	16.648155	11.453244		
Pt	15.495739	13.377876	8.146674		
Pt	14.979707	15.395018	6.156489		
Pt	16.251143	16.047901	8.314393		
Pt	12.685162	13.821604	13.299468		
Pt	14.928603	13.171079	11.912530		
Pt	12.592945	13.903094	8.267067		
Pt	13.619905	16.445446	8.177944		
Pt	17.255566	15.734431	10.827896		
Pt	15.002684	11.433585	9.824730		
Pt	16.985621	13.100601	10.300483		
Pt	15.387600	15.649900	12.792526		
Pt	11.913689	14.347262	10.817612		
Pt	14.472786	14.861400	10.052364		
Pt	13.828308	13.095462	6.073807		

IS on Pt₁₅O₄@CNT: (in total 21 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)			28.0000	28.0000	29.3063
90.0000	90.0000	90.0000			
O	8.660405	6.880276	10.247208		
O	7.363454	7.064240	10.751048		
O	10.825159	9.887857	14.059969		
O	8.735659	10.218730	9.204498		
O	7.308237	7.378442	19.533646		
O	10.633768	9.143555	19.388582		
Pt	7.031168	8.653988	18.010508		
Pt	9.194503	7.839969	19.533185		
Pt	9.842457	7.847902	11.526547		
Pt	10.532201	9.798185	9.835311		
Pt	7.015063	10.589938	13.354784		
Pt	7.642718	10.153817	10.822316		
Pt	9.627952	10.344428	12.442935		
Pt	7.237708	8.858522	15.365085		
Pt	9.824298	8.030569	14.207676		

Pt	9.380724	10.546395	15.315254
Pt	9.645377	10.027228	17.885803
Pt	7.421567	8.098967	12.532162
Pt	9.262379	7.620374	16.760856
Pt	7.417805	11.065479	16.964567
Pt	7.861668	6.428790	14.709665

TS on Pt₁₅O₄/CNT: (in total 21 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	16.211902	14.966544	5.421950
O	17.058496	13.526312	6.441345
O	17.383161	15.489124	12.931411
O	13.443775	15.680283	13.404200
O	18.121239	16.336821	9.323662
O	12.932173	17.581274	9.909726
Pt	13.241934	16.602137	11.542683
Pt	15.926718	13.380883	7.944567
Pt	14.653113	15.216950	6.427405
Pt	16.360324	16.080529	8.471668
Pt	12.680469	13.793715	13.322580
Pt	14.974760	13.074910	12.060901
Pt	12.719413	13.947708	8.206751
Pt	13.686918	16.519544	8.419985
Pt	17.261491	15.802401	10.989489
Pt	14.936569	11.635594	9.760419
Pt	17.018008	13.166689	10.388507
Pt	15.429024	15.569728	12.922019
Pt	12.137251	14.264594	10.773708
Pt	14.648182	14.714164	10.095315
Pt	13.980162	12.681370	6.170795

TS on Pt₁₅O₄@CNT: (in total 21 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)	28.0000	28.0000	29.3063
90.0000 90.0000 90.0000			
O	8.243730	7.199562	10.009755
O	6.961245	8.035940	10.635495
O	10.797835	9.796186	13.921208
O	9.394584	10.426493	9.308626
O	7.296887	7.411481	19.410708
O	10.641651	9.181701	19.378782
Pt	7.076050	8.660657	17.847075
Pt	9.172080	7.913343	19.493075
Pt	9.604261	7.418384	11.450605
Pt	10.908417	9.430189	10.139767
Pt	6.898509	10.501851	12.956131
Pt	7.868698	9.894372	10.399386
Pt	9.507587	10.105063	12.370625
Pt	7.239672	8.993577	15.225479
Pt	9.782718	7.962081	14.165642
Pt	9.451351	10.533167	15.246958
Pt	9.722527	10.059945	17.821556
Pt	7.341279	7.912751	12.675150
Pt	9.338236	7.638661	16.745570
Pt	7.486027	11.106563	16.904992
Pt	7.794363	6.436082	14.849347

IS on Pt₁₅O₆/CNT: (in total 23 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)				28.0000	28.0000	29.3063
90.0000	90.0000	90.0000				
O	17.233702	11.332849	12.362075			
O	16.007145	11.366262	13.060732			
O	14.886714	14.145051	4.715258			
O	16.042101	11.415376	8.113054			
O	17.379900	15.395178	12.909889			
O	13.457806	15.715800	13.194259			
O	18.481143	15.897208	9.300274			
O	13.239020	17.296063	9.470089			
Pt	13.387548	16.478016	11.215478			
Pt	16.570779	13.284614	8.301849			
Pt	15.543296	14.792530	6.414541			
Pt	16.712170	15.945237	8.428552			
Pt	12.707486	13.808465	13.298059			
Pt	15.021397	12.954813	12.177663			
Pt	12.867965	13.808195	8.186424			
Pt	14.074623	16.220550	8.041305			
Pt	17.505362	15.366521	10.946916			
Pt	14.890502	11.651649	9.761086			
Pt	17.205917	12.699803	10.884420			
Pt	15.449936	15.559828	12.748445			
Pt	12.326360	14.086924	10.738812			
Pt	14.857120	14.570271	10.032219			
Pt	13.854434	12.811521	5.811430			

IS on Pt₁₅O₆@CNT: (in total 23 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)				28.0000	28.0000	29.3063
90.0000	90.0000	90.0000				
O	7.282818	9.757057	19.842400			
O	7.811891	10.944317	19.506443			
O	10.619899	9.990696	13.766887			
O	8.245355	10.934572	9.005739			
O	7.529647	7.141068	19.424700			
O	10.752357	9.086118	19.256240			
O	6.596667	8.165495	11.083326			
O	10.431783	7.909274	9.732767			
Pt	7.134322	8.624569	18.020459			
Pt	9.366665	7.732287	19.414336			
Pt	10.256283	7.509751	11.731163			
Pt	9.641191	9.594546	9.383884			
Pt	7.057744	10.508269	13.127774			
Pt	7.265904	9.883671	10.408453			
Pt	9.570717	10.108103	12.026418			
Pt	7.216455	8.890774	15.351573			
Pt	9.849873	8.057053	14.257697			
Pt	9.231420	10.626476	15.123891			
Pt	9.877992	9.983067	17.697319			
Pt	7.738151	7.932585	12.636033			
Pt	9.316350	7.569926	16.768422			
Pt	7.554588	11.032235	17.080949			
Pt	7.887628	6.403018	14.827714			

TS on Pt₁₅O₆/CNT: (in total 23 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)			28.0000	28.0000	29.3063
90.0000	90.0000	90.0000			
O	17.488811	11.260842	11.967240		
O	15.726766	11.344454	13.042452		
O	14.892184	14.151033	4.735563		
O	15.988523	11.444149	8.162566		
O	17.377470	15.510969	12.909279		
O	13.443634	15.728266	13.208973		
O	18.488388	15.925822	9.295179		
O	13.243708	17.306339	9.493128		
Pt	13.378054	16.498612	11.241543		
Pt	16.560384	13.303544	8.330862		
Pt	15.534700	14.788806	6.441908		
Pt	16.714991	15.953783	8.436401		
Pt	12.723903	13.811609	13.290756		
Pt	15.150628	12.990034	12.351493		
Pt	12.852183	13.806217	8.189944		
Pt	14.079423	16.203440	8.089556		
Pt	17.501667	15.420976	10.945936		
Pt	14.884339	11.678297	9.837070		
Pt	17.247173	12.753728	10.905137		
Pt	15.441668	15.599885	12.761052		
Pt	12.295449	14.117076	10.735617		
Pt	14.843992	14.548776	10.090036		
Pt	13.851225	12.809235	5.816569		

TS on Pt₁₅O₆@CNT: (in total 23 atoms)

Lattice Parameters (a, b, c, alpha, beta and gamma)			28.0000	28.0000	29.3063
90.0000	90.0000	90.0000			
O	8.692630	10.942325	19.372766		
O	6.884111	9.876265	19.384578		
O	10.653819	9.977866	13.716210		
O	8.295520	10.958655	8.990522		
O	7.708695	7.195931	19.407095		
O	10.735067	9.110183	19.282735		
O	6.642938	8.146933	10.983258		
O	10.451060	7.917650	9.698720		
Pt	7.271084	8.674048	17.973921		
Pt	9.572430	7.601588	19.319086		
Pt	10.161124	7.460493	11.649360		
Pt	9.686808	9.615811	9.359647		
Pt	7.010779	10.475012	13.076462		
Pt	7.287713	9.905695	10.368875		
Pt	9.490550	10.097313	12.039633		
Pt	7.223142	8.847609	15.274254		
Pt	9.858948	8.056169	14.169008		
Pt	9.321843	10.544247	15.167541		
Pt	9.526845	10.125331	17.872236		
Pt	7.669392	7.872185	12.603262		
Pt	9.490497	7.607190	16.715776		
Pt	7.314250	11.073127	16.723048		
Pt	7.940790	6.397593	14.823571		