Supporting Information for: Revealing the Adsorption Mechanisms of Nitroxides on Ultra-Pure, Metallicity-Sorted Carbon Nanotubes

Georgina Ruiz-Soria,[†] Alejandro Pérez Paz,[‡] Markus Sauer,[†] Duncan John Mowbray,[‡] Paolo Lacovig,[¶] Matteo Dalmiglio,[¶] Silvano Lizzit,[¶] Kazuhiro Yanagi,[§] Angel Rubio,[‡] Andrea Goldoni,[¶] Paola Ayala,[*,†] and Thomas Pichler[*,†]

[†] Faculty of Physics, University of Vienna, Strudlhofgasse 4, A-1090 Vienna, Austria
[‡] Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, Universidad del País Vasco UPV/EHU, E-20018 San Sebastián, Spain
[¶] Sincrotrone Trieste, s.s. 14 km 163.5, 34149 Trieste, Italy
[§] Department of Physics, Tokyo Metropolitan University, Hachioji, 192-0397 Tokyo, Japan

Contents

1. Samples

The single-walled carbon nanotubes (SWCNTs) used in our experiments are material in which semiconducting and metallic separation has been achieved, allowing the formation of high-purity networks.[S1] The overall morphology of these films can be observed in the scanning electron microscopy (SEM) micrograph shown in Fig. S1. This image corresponds to the semiconducting sample but there is no observable difference between both types of films with this imaging technique.

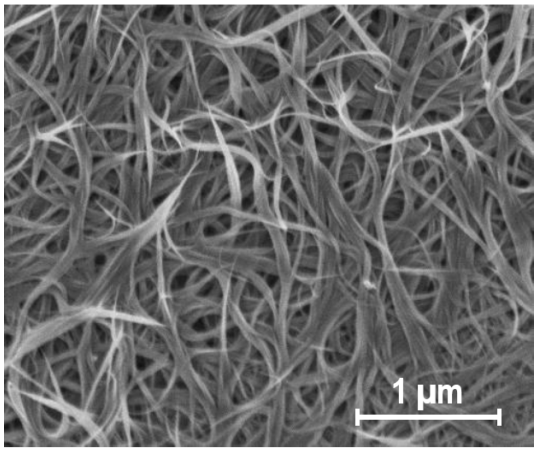

Figure S1. Scanning Electron Microscopy micrograph at intermediate magnification showing the overall morphology of the nanotube films used in the experiments.

Both types of samples were purified and separated into metallic and semiconducting tubes. They were then deposited on sapphire substrates.[S2,S3] In our previous studies on these kinds of samples, we have shown that the SWCNT buckypapers have less than 1 wt% of processing residuals with X-ray photoelectron spectroscopy (XPS), with negligible residual magnetic metal impurity content. Typically, in these samples the remaining amount of surfactants, such as deoxycholate sodium salt, is below the detection limit of XPS and Fourier transform infrared spectroscopy (FT-IR). The G/D ratio in the Raman spectra of these SWCNT samples is typically around 20 from previous studies.[S2,S3] As seen in the optical absorption spectra of these high purity samples (metal and semiconducting) shown in Fig. S2, no bands associated with the other conduction type are identified in either spectra.

Other spectroscopy studies that prove the high purity of the samples can be done with photoemission and X-ray absorption spectroscopy, and in particular valence band photoemission. These studies would be useless in the presence of impurities using a macroscopic sample, as can be understood from some previous publications.[S4–S7]

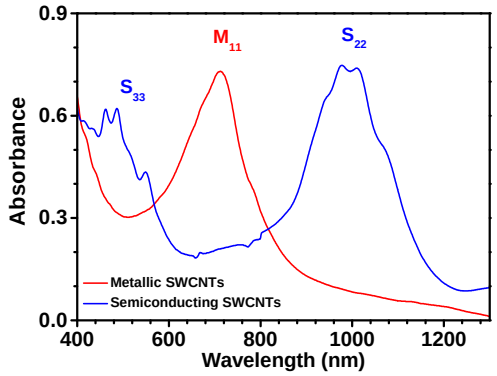

Figure S2. Optical absorption spectra of of the high purity samples: metallic (red) and semiconducting (blue).

Additionally, our previous reports on these type of nanotube networks have confirmed their ultra-high purity with other techniques. For instance, it is now understood how the presence of semiconducting species affects the conduction mechanisms in SWCNT–networks. The transport mechanisms systematically change as the

relative content of metallic to semiconducting SWCNTs is varied and quantum transport was achieved only in macroscopic networks of pure metallic SWCNTs.[S2]

2. Simulated C 1*s* Spectra

Table S1. Carbon Species, Isolated Gas Phase Molecules, and Functional Groups Studied.

C Species	Molecule	Formula	Group
O=C=O	carbon dioxide	CO_2	
C≡O	carbon monoxide	CO	
C=O	ethenone	CH_2CO	ketene
	formaldehyde	CH_2O	aldehyde / carbonyl
	acetyl radical	CH_3CO	acetyl
	acetone	$(CH_3)_2CO$	ketone / carbonyl
C–O	phenol	C_6H_5OH	hydroxyl
	ethylene oxide	C_2H_4O	epoxide
C–N	nitrobenzene	$C_6H_5NO_2$	nitro
	pyridine-N-oxide	C_5H_5NO	amine oxide
	pyridine	C_5H_5N	pyridyl

2.1. Isolated Gas Phase Species. Core-level shifts provide an electronic "fingerprint" of the local chemical environment of an atomic species. This is due to the high degree of localization of these nearly-atomic levels, such as the C 1*s*. For this reason, simulated C 1*s* spectra for molecular species may be used to obtain a "blueprint" of the expected core-level shifts for various atomic species (C≡O, C=O, C–O, C–N) within representative functional groups (ketene, carbonyl, acetyl, hydroxyl, epoxide, nitro, amine oxide, pyridyl, etc.). Thus, to obtain further insight into the possible functional groups that may be present in the experimental SWCNT samples we have simulated the C 1*s* spectra for the representative molecules listed in Table S1 in gas phase.

To this end, we have employed more than 6 Å of vacuum and non-periodic boundary conditions in all directions. In this way, we ensure a common vacuum-level reference between the all-electron C 1*s* eigenenergies calculated for the various molecular species in Table S1. The C 1*s* spectra is then simulated by employing a Lorentzian broadening with an inverse lifetime of 0.27 eV, and aligning the calculated and experimental C 1*s* levels of the C–C species in acetone, as shown in Fig. S3.

Comparison of the simulated C 1*s* spectra in Fig. S3 with the high binding energy feature in the XPS C 1*s* spectra for SWCNTs dosed with NO_2 clearly indicates this feature is due to a C=O species, as both C–O and C–N shifts are too small. Further, the core-level shift arising from a ketene group yields the largest shift, and is well separated from the carbonyl and acetyl groups. This provides further verification that this feature oberved in the XPS C 1*s* spectra is due to a C=O species in a ketene group on a SWCNT.Furthermore, the good matching shown in Fig. S3 between calculated and experimental XPS spectra for acetone (red squares)[S8] validates our computational approach.

2.2. Oxygen on SWCNTs. To further justify our assignment of the feature observed in the XPS C 1*s* spectra at high binding energy to the C=O species of a ketene group, we have performed further calculations for the C=O species of a carbonyl group and C–O species of epoxide and chemisorbed O_2. Since core states are highly localized, we can investigate the effect of several functional groups within the same calculation. In this way, we can ensure a common reference between calculations. The optimized geometries, C 1*s* levels, and simulated spectra for a carbonyl group adsorbed on a carbene site of a monovacancy, an epoxide group adsorbed on a pentagon adjacent to a monovacancy, and an O_2 molecule adsorbed on a semiconducting (10,0) and metallic (6,6) SWCNT are shown in Fig. S4. For both types of SWCNT, we find the C=O species of a carbonyl group and C–O species are at too weak binding energy to give rise to the experimentally observed feature. However, it should be noted that the presence of carboxyl and epoxide groups in the experimental spectra cannot be ruled out as their signals may appear in the region between the main and ketene peaks.

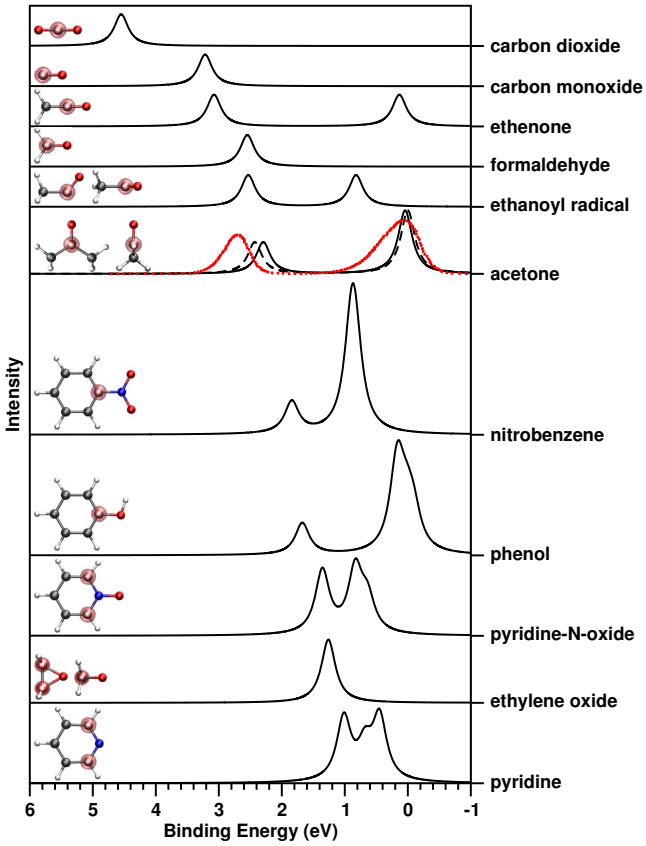

Figure S3. Simulated C 1*s* core-level shifts in eV relative to the C 1*s* level of the C–C species in acetone for various molecular species. Schematics of each molecule and isosurfaces (0.11 $e/Å^{3/2}$) of the most strongly bound C 1*s* level are shown as insets. H, C, N, and O atoms are depicted as white, gray, blue, and red spheres, respectively. For acetone, simulated C 1*s* core-level shifts for the experimental geometry (**- - -**) and XPS C 1*s* measurements (■) are also provided.

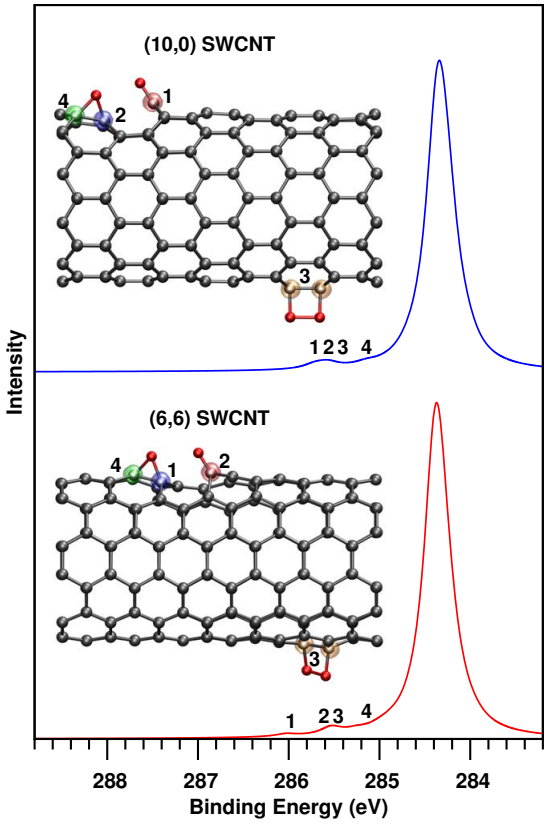

Figure S4. Simulated C 1*s* spectra for defective semiconducting (10,0) (top) and metallic (6,6) (bottom) SWCNTs with adsorbed molecular oxygen (orange), epoxide (blue and green), and carbonyl (red) groups. Schematics of each system and isosurfaces (0.11 $e/\text{Å}^{3/2}$) of the four most strongly bound C 1*s* levels are shown as insets. C and O atoms are depicted as gray and red spheres, respectively.

3. Calculated Geometries and Total Energies

All geometries were optimized within the local density approximation (LDA)[S9] until a maximum force less than 0.05 eV/Å was obtained. The total energy for the relaxed structure is given in Hartrees. All coordinates (provided in xyz format below) and cell dimensions are given in Å. For the acetone molecule, we also provide the experimental geometry and its corresponding LDA energy in Table S8.

3.1. Isolated Gas Phase Species.

Table S2. Coordinates in Å of carbon dioxide
***E* = -188.4210 Ha**

```
3
carbon dioxide cell=[12.8, 12.8, 14.4]
C   6.400000   6.400000   7.200000
O   6.400000   6.400000   8.376975
O   6.400000   6.400000   6.023025
```

Table S3. Coordinates in Å of carbon monoxide
***E* = -113.0620 Ha**

```
2
carbon monoxide cell=[12.8, 12.8, 13.6]
O   6.400000   6.400000   7.339014
C   6.400000   6.400000   6.205357
```

Table S4. Coordinates in Å of ethenone
***E* = -152.0299 Ha**

```
5
ethenone cell=[14.4, 15.2, 12.8]
C   7.200000   6.629969   6.400000
O   7.200000   9.109202   6.400000
H   8.145708   6.091162   6.400000
H   6.254292   6.091162   6.400000
C   7.200000   7.937511   6.400000
```

Table S5. Coordinates in Å of formaldehyde
***E* = -114.2274 Ha**

```
4
formaldehyde cell=[14.4, 14.4, 12.8]
C   7.200000   6.886825   6.400000
O   7.200000   8.099027   6.400000
H   8.153556   6.298014   6.400000
H   6.246445   6.298014   6.400000
```

Table S6. Coordinates in Å of acetyl radical
***E* = -152.5804 Ha**

```
6
acetyl radical cell=[14.4, 13.6, 15.2]
O   7.186157   6.658713   9.023855
C   7.192034   5.998570   8.033677
C   7.191491   6.440020   6.620282
H   7.190326   7.545179   6.553618
H   6.305273   6.023357   6.120142
H   8.075547   6.018981   6.121409
```

Table S7. Coordinates in Å of acetone
***E* = -192.2195 Ha**

```
10
acetone cell=[14.4, 16.8, 15.2]
O   7.194479   8.388653   9.005765
C   7.197208   8.395448   7.781195
C   7.195155   9.660136   6.987924
H   7.191535  10.535616   7.648972
H   6.312782   9.689635   6.326095
H   8.072519   9.697749   6.320201
C   7.197111   7.139395   6.975212
H   6.336770   7.128990   6.284221
H   7.164178   6.254686   7.622547
H   8.094251   7.099335   6.334092
```

Table S8. Experimental coordinates in Å of acetone
***E* = -192.2169 Ha**

```
10
acetone cell=[14.4, 16.8, 15.2]
C   7.310400   9.394500   6.841100
C   7.491400   8.438600   8.012200
C   7.346500   6.949100   7.732400
O   7.744600   8.853300   9.139900
H   6.308700   9.296400   6.423600
H   8.039000   9.179100   6.060100
H   7.448600  10.425900   7.166300
H   6.354100   6.732400   7.338200
H   8.091300   6.626100   7.005600
H   7.486600   6.374100   8.648000
```

Table S9. Coordinates in Å of nitrobenzene
***E* = -434.6593 Ha**

14
nitrobenzene cell=[17.6, 18.4, 12.8]

C	9.423058	11.092330	6.400000
C	10.196996	9.942475	6.400000
C	9.587988	8.700289	6.400000
C	8.206024	8.641131	6.400000
C	7.417426	9.778537	6.400000
C	8.037533	11.011347	6.400000
N	7.560735	7.345418	6.400000
O	8.294843	6.333715	6.400000
O	6.311257	7.317178	6.400000
H	9.913310	12.069673	6.400000
H	11.288687	10.008559	6.400000
H	10.149964	7.762432	6.400000
H	6.332306	9.665477	6.400000
H	7.442444	11.927286	6.400000

Table S10. Coordinates in Å of phenol
***E* = -305.6367 Ha**

13
phenol cell=[17.6, 12.8, 16.8]

H	10.321216	6.457342	10.546109
C	9.781573	6.420628	9.596916
C	10.476565	6.404482	8.400232
H	11.567680	6.415058	8.399552
C	9.778830	6.382661	7.202859
H	10.319727	6.354709	6.253665
C	8.396528	6.378600	7.194566
H	7.830579	6.340255	6.259849
C	7.708230	6.394464	8.397673
C	8.396972	6.415458	9.600285
H	7.843188	6.448025	10.545886
O	6.328415	6.383233	8.320459
H	6.033467	6.423246	9.267341

Table S11. Coordinates in Å of pyridine-N-oxide
***E* = -321.5779 Ha**

12
pyridine-N-oxide cell=[17.6, 16.8, 12.8]

C	10.227455	8.422011	6.399837
C	9.570291	7.219522	6.401303
C	8.185029	7.184543	6.401162
C	7.505801	8.392385	6.400469
C	8.191833	9.579328	6.399165
N	9.553038	9.606006	6.398242
O	10.183576	10.737416	6.396520
H	11.311465	8.542908	6.400213
H	10.157848	6.299433	6.404773
H	7.645358	6.237603	6.403748
H	6.413689	8.424233	6.402278
H	7.735051	10.569441	6.398282

Table S12. Coordinates in Å of ethylene oxide
***E* = -153.1918 Ha**

7
ethylene oxide cell=[15.2, 14.4, 13.6]

C	6.871610	7.204511	6.290753
O	7.598001	7.232259	7.548895
H	6.338607	6.269248	6.085070
H	6.334459	8.129167	6.051221
H	8.862771	6.269634	6.093454
H	8.865648	8.130823	6.059390
C	8.328846	7.205117	6.294901

Table S13. Coordinates in Å of pyridine
***E* = -246.3191 Ha**

11
pyridine cell=[17.6, 16.8, 12.8]

C	10.154700	8.430686	6.400000
C	9.506548	7.207144	6.400000
C	8.123921	7.196973	6.400000
C	7.443965	8.403151	6.400000
C	8.186882	9.574961	6.400000
N	9.514442	9.595633	6.400000
H	11.248960	8.479876	6.400000
H	10.079243	6.276600	6.400000
H	7.573236	6.251999	6.400000
H	6.351508	8.439459	6.400000
H	7.679768	10.548184	6.400000

3.2. NO_2+SWCNTs.

Table S14. Coordinates in Å of 10NO_2+(10,0) SWCNT
***E* = -5063.4424 Ha**

110
10NO2+(10,0)SWCNT cell=[18.4, 18.4, 8.526]

C	13.103979	9.239358	3.573268
C	12.858184	10.462853	2.855687
C	12.871104	10.450255	1.426819
C	12.292948	11.533214	0.705956
C	12.291478	11.512670	3.555317
C	11.551479	12.577802	2.844896
C	11.419439	12.391310	1.390823
C	10.322639	12.897152	0.691189
C	10.292514	12.917153	3.543892
C	9.104972	13.052075	2.834361
C	9.085387	13.054573	1.405698
C	7.903583	12.873994	0.704508
C	7.891812	12.866979	3.555010
C	6.791008	12.331201	2.869306
C	6.653283	12.518747	1.415420
C	5.929910	11.433881	0.714919
C	5.955888	11.462004	3.569839
C	5.426768	10.329695	2.850136
C	5.436346	10.345826	1.421982
C	5.244456	9.132624	0.701441
C	5.251118	9.151334	3.549815
C	5.227259	7.852298	2.841877
C	5.432109	7.925007	1.386090
C	6.024409	6.872238	0.684966
C	6.070211	6.856585	3.537620
C	6.958750	6.065877	2.828040
C	6.950897	6.042896	1.401202
C	8.023970	5.519526	0.692645
C	8.066309	5.516087	3.545262
C	9.258160	5.310363	2.854277
C	9.247580	5.105125	1.401869
C	10.464648	5.520465	0.685522
C	10.465084	5.515347	3.550196
C	11.550324	6.082839	2.834753
C	11.534973	6.124736	1.412806
C	12.391417	6.969922	0.711737
C	12.400292	6.948591	3.559685
C	12.968934	8.043234	2.875397
C	13.188629	7.982102	1.422864
C	13.138934	9.283990	0.722096
C	13.132684	9.283543	7.837702
C	12.919323	10.472471	7.137013
C	13.121943	10.544195	5.678937
C	12.272089	11.528040	4.970708
C	12.299393	11.525403	7.820896
C	11.386826	12.348467	7.100465
C	11.402883	12.339326	5.671041
C	10.291646	12.906606	4.951377
C	10.326883	12.898931	7.807294
C	9.095038	13.322947	7.105793
C	9.101634	13.091229	5.652072
C	7.900159	12.868088	4.965212
C	7.882133	12.864411	7.817982
C	6.827448	12.306216	7.115345
C	6.818022	12.290757	5.686636
C	5.953511	11.467949	4.976535
C	5.934792	11.436007	7.831855
C	5.387354	10.360430	7.131935
C	5.166130	10.427797	5.676324
C	5.254975	9.129872	4.965696
C	5.245707	9.145068	7.815926
C	5.490058	7.943472	7.094698
C	5.491330	7.961861	5.665606
C	6.077578	6.861285	4.949240
C	6.026228	6.876282	7.800385
C	6.796761	5.829978	7.096898
C	6.934674	6.018236	5.648983
C	8.055422	5.504585	4.965769
C	8.040330	5.504404	7.812355
C	9.237887	5.352943	7.112836
C	9.253856	5.317288	5.690602
C	10.465774	5.510267	4.976968
C	10.455168	5.513935	7.841034
C	11.687646	5.905013	7.127931
C	11.557244	6.061908	5.672466
C	12.381882	6.948402	4.980064
C	12.401124	6.986174	7.832658
C	12.924725	8.057201	7.122157
C	12.907855	8.067445	5.695989
C	13.107473	9.238725	4.984472
N	9.050969	14.991482	7.167179
O	10.127217	15.529337	7.071566
O	7.951927	15.480055	7.251743
N	12.540348	13.941142	2.928208
O	13.721240	13.715673	3.018993
O	11.964697	14.997316	2.843685
N	14.661701	11.136631	5.556480
O	15.529008	10.304072	5.439924
O	14.759807	12.336267	5.630089
N	12.729488	4.571236	7.223681
O	12.187426	3.496533	7.293900
O	13.902903	4.841264	7.174470
N	14.791341	7.433008	1.340846
O	14.923683	6.237818	1.267897
O	15.629148	8.298544	1.397425
N	9.220716	3.390945	1.325045
O	8.145471	2.896902	1.547391
O	10.281705	2.870663	1.094029
N	5.813488	4.429131	7.171326
O	4.673776	4.598514	6.817428
O	6.360241	3.426187	7.552793
N	3.643512	7.304326	2.952321
O	2.800813	8.166220	2.971389
O	3.513974	6.105191	2.962416
N	3.576094	10.893697	5.590000
O	3.386427	12.083525	5.519854
O	2.770852	9.995532	5.652510
N	5.680725	13.873047	1.336841

O	6.270010	14.924344	1.265335
O	4.493972	13.666454	1.399187

Table S15. Coordinates in Å of $12NO_2$+(6,6) SWCNT
***E* = -6076.6786 Ha**

132
12NO2+(6,6)SWCNT cell=[23.2, 23.2, 9.845]

C	13.292307	9.133371	1.855637
C	13.074585	10.528222	1.853716
C	12.790702	11.177528	0.623966
C	11.901133	12.277924	0.622594
C	11.323747	12.688151	1.853863
C	10.002506	13.188566	1.854595
C	9.297836	13.271190	0.622976
C	7.902139	13.041768	0.624096
C	7.253976	12.757461	1.854855
C	6.148872	11.876000	1.856060
C	5.730489	11.304742	0.625870
C	5.229376	9.983384	0.627148
C	5.163176	9.279158	1.858609
C	5.397728	7.886933	1.859530
C	5.680371	7.236031	0.628226
C	6.577626	6.143123	0.629573
C	7.147993	5.724059	1.859627
C	8.463016	5.207268	1.859172
C	9.167857	5.131332	0.629026
C	10.563943	5.349870	0.627964
C	11.210241	5.639718	1.858668
C	12.303952	6.532476	1.857865
C	12.730195	7.102584	0.625631
C	13.216479	8.431812	0.625796
C	13.292292	9.133611	4.317576
C	13.075034	10.528721	4.316932
C	12.799053	11.183371	3.084834
C	11.896914	12.274291	3.083413
C	11.323512	12.686343	4.313469
C	10.001930	13.181580	4.312880
C	9.297924	13.259725	3.084199
C	7.900107	13.042571	3.085436
C	7.252805	12.754233	4.316740
C	6.144598	11.877375	4.317409
C	5.724846	11.307504	3.086416
C	5.228903	9.983868	3.088341
C	5.164614	9.279145	4.318883
C	5.399963	7.886916	4.318640
C	5.688035	7.240427	3.089053
C	6.575956	6.139718	3.090450
C	7.148128	5.722781	4.321380
C	8.463154	5.206461	4.320700
C	9.167246	5.121614	3.089862
C	10.563337	5.346817	3.088639
C	11.209076	5.639055	4.318317
C	12.301544	6.533188	4.315613
C	12.719768	7.106544	3.086656
C	13.224584	8.428017	3.087150
C	13.292546	9.133442	6.777681
C	13.074492	10.528177	6.776227
C	12.789737	11.177066	5.546327
C	11.901076	12.276825	5.544966
C	11.323609	12.686401	6.776402

C	10.002267	13.181462	6.777735
C	9.296733	13.266148	5.545492
C	7.901023	13.033230	5.546358
C	7.252951	12.754192	6.777029
C	6.144612	11.877752	6.778251
C	5.725395	11.306919	5.547889
C	5.229698	9.983571	5.549601
C	5.165988	9.279048	6.781037
C	5.400171	7.887090	6.781951
C	5.683626	7.236401	5.550554
C	6.578817	6.141931	5.551480
C	7.148381	5.723922	6.782413
C	8.463524	5.209922	6.781715
C	9.167451	5.129927	5.551367
C	10.563328	5.347969	5.550286
C	11.209144	5.641564	6.781162
C	12.301990	6.534165	6.780274
C	12.728482	7.103082	5.547552
C	13.215440	8.432182	5.547746
C	13.293491	9.133309	9.240323
C	13.075812	10.528919	9.239581
C	12.798373	11.182722	8.007509
C	11.897601	12.274447	8.006641
C	11.324384	12.688413	9.236337
C	10.002807	13.187805	9.236565
C	9.298300	13.258724	8.006692
C	7.900684	13.042022	8.007585
C	7.254151	12.756995	9.239266
C	6.148967	11.876390	9.241016
C	5.722796	11.309051	8.009999
C	5.230936	9.983254	8.010851
C	5.164540	9.278932	9.240929
C	5.397543	7.886574	9.241130
C	5.687847	7.240512	8.011874
C	6.575974	6.140685	8.013106
C	7.148527	5.725647	9.244516
C	8.463490	5.211269	9.244320
C	9.167812	5.124014	8.013091
C	10.563901	5.351141	8.011826
C	11.209830	5.641839	9.240953
C	12.304011	6.533440	9.238342
C	12.719912	7.107230	8.009006
C	13.225009	8.428402	8.009575
N	9.202342	15.843000	5.541006
O	10.250542	16.423902	5.603779
O	8.069974	16.220276	5.412469
N	9.176678	16.015384	0.615710
O	10.174037	16.674244	0.710501
O	8.016048	16.306298	0.512746
N	15.020743	12.630075	8.005518
O	16.084033	12.081158	8.095407
O	14.697305	13.783728	8.094761
N	15.000170	12.613162	3.082816
O	16.041642	12.023090	3.161002
O	14.714885	13.776212	3.174303
N	15.053593	6.023530	5.538741
O	15.126992	4.830306	5.632199
O	15.887538	6.884158	5.434910
N	15.049048	5.981796	0.615705
O	15.101548	4.786956	0.703899
O	15.897056	6.825981	0.501310
N	9.167000	2.390463	8.000847
O	8.163565	1.740460	8.100175
O	10.323296	2.088857	7.892743
N	9.194982	2.204326	3.078190
O	8.223536	1.507620	3.173993
O	10.366586	1.964656	2.974452
N	3.386500	5.777684	5.540286
O	2.308573	6.293995	5.644720
O	3.729602	4.631280	5.434814
N	3.397309	5.799753	0.615768
O	2.309249	6.295365	0.715154
O	3.764434	4.660665	0.512564
N	3.224740	12.581400	8.000277
O	3.066541	13.765349	8.098616
O	2.462623	11.663671	7.858037
N	3.232512	12.753292	3.076965
O	3.058450	13.936165	3.144308
O	2.485182	11.818574	2.972662

3.3. O+SWCNTs.

Table S16. Coordinates in Å of O+(10,0) SWCNT ketene group
***E* = -6125.6211 Ha**

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O+(10,0)SWCNT cell=[19.2, 19.2, 17.0520]

C	5.927858	10.983826	3.522052
C	5.551819	9.815449	2.808698
C	5.550596	9.811901	1.391866
C	5.527142	8.583964	0.680518
C	5.531837	8.591293	3.523839
C	5.912728	7.425496	2.809601
C	5.910673	7.421525	1.395516
C	6.678827	6.465681	0.679494
C	6.685674	6.474548	3.525670
C	7.744450	5.857713	2.809616
C	7.741491	5.854528	1.395053
C	8.947613	5.645131	0.679913
C	8.952890	5.648872	3.523377
C	10.163867	5.830719	2.808360
C	10.161452	5.829935	1.391199
C	11.269900	6.350270	0.674572
C	11.278112	6.346774	3.520944
C	12.209755	7.142309	2.802878
C	12.202663	7.152776	1.382120
C	12.875064	8.178546	0.665718
C	12.898553	8.153351	3.519972
C	13.271544	9.324687	2.806700
C	13.267335	9.339260	1.388258
C	13.294195	10.576253	0.691970
C	13.278038	10.543230	3.532078
C	12.902101	11.714323	2.832688
C	12.924973	11.732917	1.431124
C	12.168767	12.727082	0.750220
C	12.123329	12.674661	3.539811
C	11.059665	13.303524	2.833147
C	11.074011	13.326641	1.431761
C	9.875269	13.522478	0.694365
C	9.847269	13.506506	3.533225
C	8.640595	13.330127	2.809352
C	8.653744	13.327318	1.390624
C	7.552345	12.789355	0.668131
C	7.527829	12.808338	3.522408
C	6.606326	12.003522	2.804656
C	6.615430	11.997438	1.383608
C	5.931327	10.974156	0.674611
C	5.925722	10.974330	7.789543
C	5.546864	9.811025	7.070520
C	5.549795	9.815779	5.653694
C	5.531839	8.591523	4.939111
C	5.526260	8.583996	7.783076
C	5.911457	7.421888	7.067726
C	5.913729	7.426363	5.653822
C	6.686462	6.474989	4.938281
C	6.680397	6.466587	7.783216
C	7.742887	5.854995	7.067909
C	7.745553	5.858140	5.653574
C	8.953066	5.648642	4.939097
C	8.948815	5.642618	7.783193
C	10.162505	5.823984	7.070629
C	10.164617	5.828317	5.653251
C	11.278322	6.344432	4.940068
C	11.273511	6.340353	7.788179
C	12.205227	7.141418	7.078873
C	12.211458	7.137350	5.657170
C	12.898776	8.149527	4.939290
C	12.874032	8.168045	7.797979
C	13.250373	9.328086	7.072079
C	13.265470	9.318691	5.657335
C	13.272612	10.541312	4.943742
C	13.255264	10.560227	7.769273
C	12.903838	11.725988	7.048716
C	12.892021	11.711217	5.646356
C	12.122769	12.673792	4.935991
C	12.168274	12.725880	7.754177
C	11.072019	13.307126	7.049798
C	11.059134	13.294285	5.647272
C	9.846815	13.501048	4.944514
C	9.868695	13.484160	7.771675
C	8.649395	13.307763	7.073426
C	8.637720	13.322382	5.658562
C	7.525390	12.807121	4.941723
C	7.548381	12.782226	7.798892
C	6.609895	11.994939	7.080459
C	6.603452	12.002868	5.658985
C	5.925811	10.983788	4.940961
C	12.713269	8.264622	12.049774
C	13.052311	9.437366	11.342922
C	13.163381	9.384759	9.929570
C	13.229806	10.580008	9.182998
C	12.989012	10.681896	12.041960
C	12.959853	11.833462	11.256221
C	12.958611	11.786886	9.860630
C	12.223335	12.789257	9.140203
C	12.517048	13.126814	11.787236
C	11.172807	13.381562	11.262165
C	11.125178	13.368545	9.864936
C	9.891915	13.460864	9.186428
C	10.025487	13.241168	12.044772
C	8.783110	13.126443	11.345522
C	8.716422	13.228197	9.931260
C	7.577257	12.750030	9.217546
C	7.663383	12.637554	12.051717
C	6.672895	11.923858	11.340816
C	6.647878	11.951966	9.923897
C	5.930900	10.962198	9.205824
C	5.942774	10.941224	12.051946
C	5.533410	9.790966	11.333618
C	5.538902	9.798483	9.916190
C	5.520832	8.577257	9.199808
C	5.503493	8.566539	12.048757
C	5.897929	7.407486	11.331122
C	5.903338	7.412792	9.915245
C	6.677823	6.463438	9.198984

C	6.671946	6.457200	12.049055
C	7.731534	5.841612	11.331802
C	7.735482	5.845930	9.915545
C	8.943552	5.636419	9.200600
C	8.936735	5.623090	12.048098
C	10.146600	5.809108	11.332649
C	10.153107	5.814615	9.915181
C	11.263097	6.341925	9.204694
C	11.240222	6.352838	12.050595
C	12.128440	7.193783	11.338686
C	12.160275	7.171739	9.922169
C	12.838688	8.192459	9.216510
C	12.827549	8.202331	16.298281
C	13.131649	9.390627	15.586476
C	12.993612	9.475211	14.176398
C	12.808841	10.718801	13.478433
C	13.237488	10.587071	16.321986
C	12.802588	11.738015	15.650705
C	12.360942	11.805653	14.301651
C	12.157633	12.714714	16.427003
C	11.094374	13.206144	15.653148
C	11.225565	12.781914	14.302960
C	10.083985	13.066510	13.481757
C	9.892819	13.467037	16.324836
C	8.722392	13.196340	15.589896
C	8.825440	13.072763	14.179313
C	7.675720	12.639824	13.463682
C	7.582250	12.742809	16.300318
C	6.650790	11.947982	15.592783
C	6.679291	11.928215	14.176429
C	5.946677	10.943479	13.465493
C	5.933582	10.960602	16.310106
C	5.541632	9.797063	15.598543
C	5.536475	9.792041	14.181702
C	5.504109	8.567229	13.466097
C	5.520756	8.576299	16.315788
C	5.902159	7.411897	15.599297
C	5.896860	7.407483	14.183460
C	6.672337	6.458074	13.465777
C	6.675767	6.461909	16.315565
C	7.734783	5.847201	15.598985
C	7.732632	5.844001	14.182607
C	8.937635	5.626141	13.465719
C	8.942273	5.639015	16.314461
C	10.150333	5.821299	15.598423
C	10.147286	5.816144	14.181092
C	11.242116	6.358983	13.464259
C	11.257708	6.351664	16.309966
C	12.152929	7.180070	15.591739
C	12.131832	7.203479	14.175330
C	12.713335	8.279373	13.461236
C	13.281143	13.925435	12.480613
O	13.974502	14.600021	13.133535

Table S17. Coordinates in Å of O+(6,6) SWCNT ketene group *E* = -6428.1889 Ha

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O+(6,6)SWCNT cell=[19.2, 19.2, 17.2287]

C	5.617579	8.643176	0.550010
C	5.618507	10.056402	0.549990
C	6.936184	12.513443	0.570897
C	8.108718	13.305196	0.585470
C	10.881305	13.528082	0.607091
C	7.034088	6.254691	0.610188
C	12.143243	12.889940	0.618034
C	13.555741	10.499288	0.640948
C	13.548922	9.085617	0.655877
C	8.293589	5.613265	0.657765
C	12.235628	6.624453	0.680194
C	11.065246	5.828402	0.686187
C	5.763478	7.974303	1.791677
C	5.770165	10.755191	1.786191
C	6.453483	11.994926	1.797987
C	6.485546	6.758940	1.817342
C	8.775436	13.539135	1.821602
C	10.185119	13.657819	1.833449
C	12.665172	12.410918	1.850769
C	13.380606	11.190930	1.863496
C	13.362626	8.407559	1.893254
C	12.686804	7.164825	1.909496
C	8.961753	5.505153	1.903883
C	10.370352	5.619965	1.917784
C	12.656500	12.399367	16.621385
C	6.476553	11.978271	16.561064
C	10.201352	5.848680	6.858396
C	8.800020	5.714220	6.864973
C	6.258863	6.732919	6.681781
C	5.560642	7.973860	6.690930
C	5.773316	10.767173	6.720478
C	6.461481	12.002061	6.729683
C	8.785183	13.544215	6.741987
C	10.194855	13.659739	6.754036
C	13.588238	10.529659	5.559159
C	13.552916	9.116119	5.573878
C	8.777335	13.548427	16.588537
C	12.123540	6.724097	5.610978
C	10.918365	5.986707	5.628576
C	8.159557	5.720823	5.589694
C	6.879352	6.302687	5.498594
C	5.464844	8.677755	5.477497
C	5.545496	10.096550	5.485320
C	6.932856	12.523013	5.499367
C	8.113993	13.303969	5.509162
C	10.889706	13.529133	5.527300
C	12.159664	12.906493	5.538562
C	10.186373	13.664206	16.601345
C	12.678253	12.424724	4.310812
C	13.400268	11.208484	4.322869
C	13.352793	8.425461	4.354514
C	12.646354	7.200967	4.374039
C	10.298670	5.696615	4.387631

C	8.894465	5.562785	4.373207
C	6.404040	6.781880	4.257540
C	5.677861	7.991261	4.243195
C	5.747006	10.771498	4.256099
C	6.448595	12.000894	4.265352
C	13.554093	10.493698	15.409027
C	8.780138	13.535751	4.281701
C	10.189800	13.655376	4.293268
C	13.565308	10.512813	3.099535
C	13.542494	9.099567	3.115738
C	12.184853	6.663922	3.148337
C	11.003478	5.886767	3.158137
C	8.234374	5.656317	3.117066
C	6.970332	6.289088	3.058648
C	5.542901	8.672281	3.011985
C	5.563418	10.086538	3.016145
C	13.558769	9.079540	15.420875
C	6.929666	12.518019	3.035530
C	8.108559	13.299751	3.047687
C	10.884606	13.527237	3.065952
C	12.151953	12.900125	3.076538
C	12.269927	6.604816	15.437545
C	11.113804	5.787313	15.444258
C	8.332935	5.537705	15.440326
C	7.078994	6.193540	15.387705
C	5.698238	8.610539	15.313306
C	13.372540	11.180335	16.634250
C	5.692780	10.020693	15.314178
C	6.953572	12.503167	15.336319
C	8.114351	13.311616	15.351896
C	10.885343	13.532817	15.376347
C	12.141484	12.885478	15.388075
C	12.658048	12.399483	14.163231
C	13.376474	11.181425	14.176187
C	13.397153	8.393577	14.191311
C	12.738799	7.138614	14.199087
C	10.468514	5.520684	14.213877
C	13.380061	8.394776	16.658411
C	9.058734	5.364680	14.231895
C	6.593666	6.674182	14.136086
C	5.931528	7.913537	14.090061
C	5.890773	10.683901	14.077336
C	6.509182	11.958526	14.097195
C	8.785513	13.563859	14.129486
C	10.194519	13.675716	14.142003
C	13.573699	10.503642	12.949160
C	13.580753	9.088718	12.959437
C	12.259540	6.624864	12.963117
C	12.722712	7.142750	16.671060
C	11.100120	5.813648	12.970075
C	8.374999	5.517532	13.033911
C	7.158485	6.193885	12.946072
C	5.855786	8.551426	12.824449
C	5.791889	9.973685	12.843498
C	6.974098	12.511371	12.881252
C	8.124868	13.330513	12.893103
C	10.891951	13.541379	12.915424
C	12.147011	12.890788	12.928761
C	12.668387	12.409919	11.702771
C	10.426178	5.562146	16.679657
C	13.397833	11.198320	11.716432
C	13.405345	8.414603	11.725662
C	12.710528	7.181854	11.729905
C	10.383181	5.687536	11.740283
C	8.993323	5.601889	11.780199
C	6.975728	6.688702	11.614990
C	6.165001	7.870158	11.574883
C	5.951522	10.688007	11.633931
C	6.530370	11.969227	11.648355
C	8.791338	13.574963	11.666926
C	9.014490	5.444371	16.675594
C	10.200188	13.682089	11.679029
C	13.597254	10.525764	10.487417
C	13.592251	9.113331	10.497136
C	12.168931	6.738126	10.496476
C	10.939840	6.053786	10.507158
C	8.113506	6.089152	10.765683
C	5.796356	8.598174	10.378447
C	5.783038	10.011551	10.403569
C	6.969750	12.523905	10.420895
C	8.125267	13.333886	10.432106
C	6.543543	6.716800	16.592858
C	10.895214	13.538728	10.452213
C	12.154599	12.897797	10.466777
C	12.680324	12.422234	9.239345
C	13.416029	11.215712	9.252231
C	13.391280	8.448810	9.263295
C	12.638963	7.260895	9.273196
C	10.131007	5.972210	9.337990
C	8.689973	5.963998	9.413549
C	5.803528	6.534557	9.016955
C	5.619648	7.965178	9.149057
C	5.833234	7.940860	16.558484
C	5.854079	10.730319	9.184534
C	6.492110	11.995047	9.192856
C	8.789191	13.565279	9.202606
C	10.199482	13.670653	9.215741
C	13.604710	10.538852	8.020350
C	13.579535	9.128169	8.030257
C	12.080560	6.780771	8.066120
C	10.831551	6.118198	8.093131
C	8.043805	5.892566	8.093947
C	6.702926	6.221806	7.914240
C	5.820990	10.725867	16.546889
C	5.485258	8.672049	7.941417
C	5.621167	10.075056	7.949813
C	6.944357	12.528424	7.962494
C	8.117962	13.318936	7.970434
C	10.894040	13.531627	7.988919
C	12.160987	12.904104	8.002186
C	12.685248	12.430206	6.773384
C	13.417562	11.220651	6.784874
C	13.356958	8.445177	6.810770
C	12.608197	7.245600	6.829775
C	5.255903	5.615995	9.777357
O	4.775702	4.786333	10.439821

Table S18. Coordinates in Å of 2O@MV (carbonyl and epoxy groups) and O_2+(10,0) SWCNT
***E* = -6313.5479 Ha**

163
O2+2O+(10,0)SWCNT cell=[19.2, 19.2, 17.0520]

C	5.977059	10.966378	3.526299
C	5.638430	9.785615	2.812664
C	5.590998	9.796298	1.398293
C	5.558430	8.578348	0.680087
C	5.660947	8.553848	3.512956
C	5.907901	7.389003	2.784930
C	5.904513	7.400801	1.386874
C	6.647883	6.419766	0.655483
C	6.443782	6.176072	3.470605
C	7.724286	5.831610	2.786253
C	7.732059	5.836602	1.382987
C	8.944579	5.672353	0.677173
C	8.910614	5.751707	3.511543
C	10.135989	5.904181	2.808744
C	10.149070	5.867930	1.395207
C	11.267059	6.374225	0.677092
C	11.261247	6.396631	3.520546
C	12.211396	7.160517	2.803903
C	12.198723	7.170128	1.381865
C	12.860683	8.206967	0.663522
C	12.915310	8.162034	3.523108
C	13.277563	9.336677	2.810302
C	13.260080	9.357672	1.386667
C	13.319381	10.592621	0.689038
C	13.291903	10.547987	3.535828
C	12.921228	11.726669	2.829384
C	12.962677	11.756152	1.441942
C	12.166714	12.730504	0.752031
C	12.119135	12.675737	3.541798
C	11.047465	13.290622	2.833626
C	11.057365	13.301938	1.431465
C	9.862888	13.501190	0.694449
C	9.839367	13.510426	3.532565
C	8.628421	13.351115	2.808714
C	8.638226	13.335687	1.392382
C	7.535525	12.799825	0.667607
C	7.516331	12.833183	3.525587
C	6.612186	12.008281	2.808442
C	6.608661	12.002013	1.385756
C	5.929017	10.976082	0.678795
C	5.928757	10.981206	7.789597
C	5.590074	9.800902	7.068206
C	5.636215	9.788574	5.654560
C	5.661594	8.555712	4.953155
C	5.563720	8.583422	7.785495
C	5.910982	7.407056	7.078197
C	5.914296	7.393689	5.680683
C	6.447973	6.179859	4.997086
C	6.657231	6.429322	7.809342
C	7.738806	5.843763	7.081471
C	7.729351	5.836085	5.680856
C	8.913891	5.752018	4.954921
C	8.951809	5.672611	7.788454
C	10.156523	5.859771	7.069170
C	10.140450	5.899717	5.655041
C	11.264836	6.392391	4.941276
C	11.281988	6.351295	7.789581
C	12.215691	7.146768	7.082404
C	12.219615	7.148911	5.658527
C	12.920043	8.154761	4.940198
C	12.890942	8.169215	7.803115
C	13.264065	9.331971	7.077451
C	13.280660	9.323563	5.660265
C	13.283737	10.544557	4.946109
C	13.266842	10.562554	7.773084
C	12.906862	11.728190	7.045891
C	12.896945	11.714529	5.650505
C	12.116940	12.672941	4.933812
C	12.158069	12.720427	7.752759
C	11.061279	13.298873	7.049969
C	11.049601	13.286513	5.646078
C	9.840141	13.507460	4.945319
C	9.860672	13.486660	7.773659
C	8.638737	13.327774	7.076734
C	8.628129	13.347030	5.662339
C	7.515193	12.833896	4.943333
C	7.534742	12.803531	7.804394
C	6.607437	12.006265	7.083471
C	6.610398	12.010655	5.659973
C	5.975197	10.968364	4.942202
O	5.489657	5.072413	3.504483
O	5.494154	5.079922	4.976442
C	12.710235	8.272018	12.052568
C	13.056495	9.439530	11.343147
C	13.170049	9.388068	9.929377
C	13.242717	10.583474	9.185814
C	13.015115	10.686907	12.041169
C	12.976722	11.850618	11.252406
C	12.960192	11.793675	9.865016
C	12.208698	12.779135	9.135638
C	12.523917	13.151997	11.789493
C	11.157788	13.339562	11.265154
C	11.113446	13.341983	9.864008
C	9.882596	13.457912	9.190187
C	10.018458	13.203401	12.047703
C	8.775356	13.104095	11.350517
C	8.707116	13.225211	9.937393
C	7.561657	12.761591	9.222592
C	7.648668	12.624422	12.055428
C	6.649326	11.929684	11.342344
C	6.629133	11.962744	9.924391
C	5.915533	10.973031	9.203312
C	5.908581	10.952877	12.053596
C	5.512002	9.796382	11.331891
C	5.529886	9.802931	9.915917
C	5.536288	8.580530	9.204110
C	5.502476	8.572888	12.047531

C	5.897252	7.413475	11.332224
C	5.902041	7.415266	9.923008
C	6.669284	6.447581	9.203972
C	6.671699	6.457187	12.054312
C	7.739987	5.846784	11.335153
C	7.744175	5.847153	9.922941
C	8.949368	5.651902	9.207016
C	8.943541	5.629134	12.048069
C	10.157310	5.800992	11.332580
C	10.163314	5.814187	9.918601
C	11.273706	6.343010	9.205485
C	11.252935	6.345868	12.050820
C	12.136032	7.188890	11.340061
C	12.171494	7.170178	9.925000
C	12.850588	8.193414	9.218806
C	12.784560	8.247143	16.300500
C	13.068877	9.448039	15.599083
C	12.908544	9.511543	14.161920
C	12.822057	10.714957	13.447719
C	13.295160	10.610246	16.326522
C	13.018235	11.880162	15.642698
C	12.547977	11.956989	14.234073
C	12.158031	12.724393	16.442956
C	11.074668	13.131866	15.666427
C	11.218799	12.781055	14.303141
C	10.082162	13.030178	13.491109
C	9.873948	13.429311	16.329323
C	8.707024	13.179126	15.588570
C	8.813304	13.046229	14.183888
C	7.660007	12.625852	13.467067
C	7.556577	12.746280	16.300912
C	6.622055	11.956008	15.596088
C	6.651252	11.932615	14.179281
C	5.909737	10.954959	13.465390
C	5.909341	10.966821	16.316554
C	5.523493	9.798785	15.601008
C	5.510834	9.796830	14.184577
C	5.501793	8.573415	13.467058
C	5.528682	8.575710	16.312512
C	5.894803	7.410749	15.591956
C	5.894068	7.412613	14.181911
C	6.670322	6.457028	13.459581
C	6.659297	6.440570	16.311657
C	7.735744	5.841937	15.591922
C	7.736165	5.844792	14.179078
C	8.941360	5.629301	13.466975
C	8.940907	5.650885	16.309175
C	10.151981	5.820581	15.597071
C	10.152486	5.806506	14.183437
C	11.248950	6.353796	13.466798
C	11.252936	6.368370	16.311075
C	12.126244	7.211302	15.594296
C	12.113140	7.217368	14.176946
C	12.683619	8.296076	13.459842
O	13.153658	13.943661	12.456675
O	13.770259	12.595181	14.654511

Table S19. Coordinates in Å of 2O@MV (carbonyl and epoxy groups) and O_2+(6,6) SWCNT
***E* = -6616.0992 Ha**

171
O2+2O+(6,6)SWCNT cell=[19.2, 19.2, 17.2287]

C	5.628423	8.660815	0.556500
C	5.609262	10.071398	0.553119
C	6.926415	12.523235	0.572765
C	8.109758	13.298254	0.587385
C	10.888281	13.552824	0.589420
C	7.058368	6.275294	0.621404
C	12.161097	12.922008	0.590748
C	13.515473	10.510458	0.641381
C	13.517741	9.096277	0.658035
C	8.303907	5.614346	0.657894
C	12.242219	6.616122	0.675591
C	11.074230	5.813328	0.677694
C	5.782631	7.995365	1.798882
C	5.746967	10.774362	1.789745
C	6.435330	12.011419	1.801155
C	6.515091	6.786493	1.826401
C	8.790735	13.500613	1.822745
C	10.200032	13.633028	1.835995
C	12.702245	12.468373	1.810947
C	13.327916	11.227323	1.856790
C	13.320332	8.424311	1.896824
C	12.678243	7.166610	1.908275
C	8.973780	5.493223	1.901672
C	10.383395	5.594852	1.913589
C	12.644305	12.395771	16.602873
C	6.464564	11.995142	16.562243
C	10.227479	5.816583	6.857073
C	8.823337	5.693572	6.864017
C	6.300680	6.762979	6.685719
C	5.595018	7.995285	6.693026
C	5.749232	10.786069	6.724817
C	6.448630	12.017228	6.730664
C	8.800816	13.517096	6.740008
C	10.212842	13.623928	6.755556
C	13.562697	10.536467	5.558020
C	13.513715	9.122798	5.572084
C	8.767781	13.559388	16.590001
C	12.137684	6.704021	5.607092
C	10.939830	5.953201	5.626935
C	8.180532	5.719503	5.588952
C	6.911241	6.323262	5.501782
C	5.479274	8.694775	5.481356
C	5.526531	10.114402	5.488917
C	6.936893	12.521889	5.499435
C	8.136888	13.267637	5.506185
C	10.929022	13.476719	5.536953
C	12.210793	12.937532	5.583076
C	10.184250	13.677244	16.602613
C	12.966675	12.634840	4.341499
C	13.413632	11.220761	4.336408
C	13.310232	8.440756	4.352808
C	12.642280	7.191400	4.369436

C	10.315090	5.666922	4.385132
C	8.910673	5.550993	4.371840
C	6.440193	6.810151	4.262533
C	5.704753	8.012733	4.248504
C	5.722261	10.790046	4.259311
C	6.436376	12.011692	4.265255
C	13.545564	10.482069	15.405336
C	8.813085	13.473027	4.276872
C	10.224831	13.589826	4.275061
C	13.496585	10.540668	3.119484
C	13.474598	9.124555	3.120088
C	12.188622	6.650011	3.145996
C	11.017256	5.855645	3.153633
C	8.251717	5.658497	3.116240
C	6.999397	6.313057	3.063614
C	5.551415	8.689948	3.016877
C	5.543277	10.104553	3.019189
C	13.568761	9.071324	15.422069
C	6.921783	12.521186	3.036863
C	8.129465	13.264256	3.048246
C	10.900485	13.543712	3.054301
C	12.345350	13.206958	3.050065
C	12.288839	6.597088	15.435172
C	11.119820	5.797534	15.439156
C	8.331563	5.529429	15.442685
C	7.074928	6.191944	15.403990
C	5.721747	8.617415	15.318729
C	13.352142	11.175038	16.628409
C	5.701930	10.027711	15.318139
C	6.942993	12.519907	15.338958
C	8.102858	13.332591	15.356044
C	10.874052	13.532513	15.368029
C	12.119069	12.869902	15.373694
C	12.633386	12.373375	14.155241
C	13.364636	11.162424	14.172015
C	13.428599	8.378476	14.191251
C	12.772476	7.122012	14.197357
C	10.468098	5.559216	14.205583
C	13.383003	8.394265	16.664157
C	9.056245	5.400824	14.215910
C	6.563512	6.657713	14.170417
C	5.966718	7.904725	14.100563
C	5.904734	10.687354	14.078445
C	6.505527	11.968120	14.100053
C	8.770089	13.586530	14.128377
C	10.181224	13.680722	14.138927
C	13.575093	10.485160	12.948671
C	13.610124	9.070502	12.959042
C	12.295189	6.614273	12.960983
C	12.735163	7.133947	16.672116
C	11.108713	5.837740	12.968929
C	8.377041	5.534231	13.024273
C	7.019026	6.012555	12.947415
C	5.896402	8.550492	12.810362
C	5.814185	9.976448	12.844611
C	6.963117	12.527337	12.881740
C	8.108824	13.355352	12.894861
C	10.876279	13.528140	12.913753
C	12.123320	12.863179	12.927046
C	12.649608	12.380513	11.705048
C	10.434857	5.557065	16.671778
C	13.390832	11.175840	11.717031
C	13.447935	8.393870	11.721134
C	12.751829	7.159869	11.726647
C	10.395375	5.727735	11.742689
C	8.998007	5.687812	11.787404
C	6.800516	6.534263	11.544862
C	6.128420	7.883566	11.573345
C	5.951872	10.694821	11.637684
C	6.519567	11.987411	11.651244
C	8.777223	13.591205	11.665266
C	9.015864	5.436444	16.665788
C	10.187890	13.678399	11.678638
C	13.606713	10.507768	10.488102
C	13.625936	9.092448	10.494127
C	12.208110	6.714966	10.492304
C	10.966078	6.045296	10.505178
C	8.128158	6.082399	10.730266
C	5.807451	8.602354	10.386969
C	5.782565	10.022310	10.410517
C	6.953523	12.542570	10.423207
C	8.114682	13.347541	10.431789
C	6.563736	6.735828	16.606604
C	10.885338	13.524868	10.455823
C	12.140796	12.872590	10.475439
C	12.672172	12.396523	9.254538
C	13.419800	11.199210	9.259968
C	13.422724	8.430240	9.256782
C	12.673514	7.235278	9.267837
C	10.164474	5.941486	9.337020
C	8.712228	5.933586	9.410669
C	5.813180	6.527966	9.009840
C	5.658506	7.971741	9.141653
C	5.853019	7.956481	16.564956
C	5.850276	10.742706	9.190012
C	6.479697	12.011038	9.195130
C	8.787505	13.559374	9.201998
C	10.195335	13.657747	9.219604
C	13.621783	10.532250	8.019100
C	13.595774	9.113925	8.027006
C	12.108500	6.754976	8.063584
C	10.860597	6.083198	8.094174
C	8.069368	5.874495	8.087636
C	6.743209	6.246687	7.917197
C	5.813147	10.737548	16.546319
C	5.514665	8.684878	7.944209
C	5.610734	10.092925	7.953655
C	6.937072	12.536698	7.960687
C	8.122728	13.311464	7.964966
C	10.896797	13.512068	7.994665
C	12.163111	12.888541	8.021491
C	12.716134	12.442662	6.801938
C	13.447739	11.223450	6.802026
C	13.354699	8.439672	6.807832
C	12.621955	7.228652	6.825648
O	5.244164	5.661065	9.650585

O	6.075437	5.420973	12.041507
O	13.231197	14.363003	3.210969
O	14.044795	13.612697	4.183458

AUTHOR INFORMATION

Corresponding Authors

paola.ayala@univie.ac.at, thomas.pichler@univie.ac.at

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