Supporting Information for

CO_2 adsorption by N-doped carbon nanotubes – a study by DFT with dispersion-correcting potentials

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Figure S1. Sample Gaussian-03 input demonstrating the use of DCPs.

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#B971 Gen OPT Pseudo=Read counterpoise=2

Methane Dimer using optimised DCPs. The monomer is also calculated with the same DCPs.

0 1
C    0.000000    1.906281    0.000000 1
H   -0.981163    1.425134    0.000000 1
H    0.553375    1.602684    0.892189 1
H    0.553375    1.602684   -0.892189 1
H   -0.125117    2.992038    0.000000 1
C    0.000000   -1.906281    0.000000 2
H    0.125117   -2.992038    0.000000 2
H    0.981163   -1.425134    0.000000 2
H   -0.553375   -1.602684    0.892189 2
H   -0.553375   -1.602684   -0.892189 2

C H 0
6-31G(d)
****

C 0
C 3 0
     F and up
 3
   2      0.08  -0.001578
   2      0.12   0.00349
   2      0.009   -0.0000042
     S - F
 1
   2      1.0      0.0
     P - F
 1
   2      1.0      0.0
     D - F
 1
   2      1.0      0.0
```

Table S2. Binding energies (kcal/mol) for training-set using B971/Basis with optimized three-function dispersion correcting potentials on carbon.

Hydrocarbon dimers	6-31G(d)[b]	STO-6G[c]	High-level[d]
$CH_4 \cdot C_6H_6$	1.14	0.79	1.23[e]
$(CH_4)_2$	0.43	0.21	0.51[f]
$CH_4 \cdot C_2H_4$	0.63	0.55	0.50[g]
P-$(C_6H_6)_2$	1.35	2.10	1.70[h]
SP-$(C_6H_6)_2$	2.30	2.18	2.63[h]
T-$(C_6H_6)_2$	2.49	1.40	2.61[h]
$(C_2H_4)_2$	1.43	0.70	1.42[f]
$(C_2H_2)_2$	1.67	0.44	1.38[i]
P-$(C_{10}H_8)_2$	3.83	4.43	3.78[j]
PC-$(C_{10}H_8)_2$	5.53	4.86	5.28[j]
T-$(C_{10}H_8)_2$	4.64	2.74	4.34[j]
TC-$(C_{10}H_8)_2$	3.38	2.39	3.09[j]
SD[a]	0.03	0.47	
%AD	11.04	32.70	
Heteroatom dimers			
HCN·HF	6.85	4.75	7.49[i]
$C_2H_4 \cdot HF$	5.19	2.23	4.50[i]
$(CF_4)_2$	0.85	0.54	0.78[k]
$(CH_3F)_2$	2.26	2.97	2.33[l]
$CH_4 \cdot HF$	1.52	0.49	1.65[g]
$CH_4 \cdot NH_3$	1.09	2.67	0.76[h]
$(CO_2)_2$	1.39	0.68	1.37[m]
$(H_2CO)_2$	3.26	2.16	3.72[i]
$H_2O \cdot C_6H_6$	3.49	1.97	3.17[n]
$(H_3CCN)_2$	5.65	3.42	6.16[l]
SD[a]	-0.04	0.94	
%AD	11.81	64.76	
SD (Total)	0.00	0.68	
%AD (Total)	11.39	47.27	

[a]Defined as the High-level value minus DCP-calculated. [b]with counterpoise corrections, $\zeta_1 = 0.08$, $c_1 = -0.001578$, $\zeta_2 = 0.12$, $c_2 = 0.00349$, $\zeta_3 = 0.009$, $c_3 = -0.0000042$. [c]$\zeta_1 = 0.06$, $c_1 = -0.0005$, $\zeta_2 = 0.12$, $c_2 = 0.004$, $\zeta_3 = 0.00725$, $c_3 = -0.000001$.[d]High-level data are generally of large basis set, CCSD(T) quality, with the exception of those for the naphthalene dimers. . [e]ref. 1. [f]ref. 2. [g]ref. 3. [h]ref. 4. [i]ref. 5. [j]ref. 6. [k]ref. 7. [l]ref. 8. [m]ref. 9. [n]ref. 10.

Table S3. Signed deviations of monomer separations (Å), relative to high-level theoretical results, for the set of non-covalently bound dimers using B971/STO-6G-DCP.

hydrocarbon dimers	Separation[a]	STO-6G	High-level[b]
$CH_4 \cdot C_6H_6$	H_4C-CM(C_6H_6)	+0.1	3.8
$(CH_4)_2$	C-C	+0.3	3.6
$CH_4 \cdot C_2H_4$	H_4C-CM(C_2H_4)	-0.3	4.2
P-$(C_6H_6)_2$	CM-CM	-0.1	3.9
SP-$(C_6H_6)_2$	CM-CM	0	3.9
T-$(C_6H_6)_2$	CM-CM	+0.2	5.0
$(C_2H_4)_2$	CM-CM	+0.2	3.8
$(C_2H_2)_2$	CM-CM	-0.2	4.3
P-$(C_{10}H_8)_2$	CM-CM	-0.1	3.8
PC-$(C_{10}H_8)_2$	CM-CM	0	3.6
T-$(C_{10}H_8)_2$	CM-CM	+0.2	5.0
TC-$(C_{10}H_8)_2$	CM-CM	0	5.2
MSD		*0*	
heteroatom dimers			
HCN·HF	N-HF	0	1.9
$C_2H_4 \cdot$HF	FH-CM(C_2H_4)	+0.1	2.2
$(CF_4)_2$	C-C	0	4.0
$(CH_3F)_2$	C-C	-0.6	3.9
$CH_4 \cdot$HF	C-HF	+0.5	2.3
$CH_4 \cdot NH_3$	C-N	-0.7	3.9
$(CO_2)_2$	C-C	+0.3	3.6
$(H_2CO)_2$	C-C	-0.2	3.6
$H_2O \cdot C_6H_6$	O-CM(C_6H_6)	0	3.4
$(H_3CCN)_2$	C-C	+0.1	3.4
MSD		*-0.1*	

[a]CM = centre-of-mass of heavy atoms [b]High-level data are generally of large basis set, CCSD(T) quality, with the exception of those for the naphthalene dimers, see Table S2 for references.

Table S4. Comparison of B971/Basis-DCP and M06-2X/6-31++G(d,p) binding energies (BE, kcal/mol) to CCSD(T)/CBS data for a series of N-containing heterocycles bound to CO_2.

Aromatic system	B971		M06-2X[a]	High-level[11]
	STO-6G	6-31G(d)[a]		
pyridine	2.55	4.01	5.14	4.46
pyrimidine	2.10	3.61	4.65	4.06
pyridazine	2.01	3.48	4.53	3.96
pyrazine	2.17	3.56	4.56	3.95
1,3,5-triazine	1.83	3.16	4.10	3.59
imidazole	2.62	4.04	5.01	4.53
2H-tetrazole	8.09	3.47	4.57	4.56
purine (BS1)	2.28	3.75	4.83	4.17
purine (BS2)	2.50	3.75	4.66	4.21
purine (BS3)	7.80	5.11	6.05	5.55
imidazopyridine	7.40	5.29	6.32	5.78
adenine	7.52	5.38	6.55	5.90
imidazopyridamine	7.28	5.58	6.79	6.12
MAD	0.36	0.51	0.53	
AD (%)	42.7	11.1	11.7	

[a]Includes counterpoise corrections.

Table S5. Calculated binding energies (kcal/mol) for C_6H_6•CO_2, C_5NH_5•CO_2 and $C_3N_3H_3$•CO_2 using various computational methods.

System[a]/Symmetry		B971-DCP		M06-2X	CCSD(T)/CBS[c]
		6-31G(d)[b]	aug-cc-pVTZ	6-31++G(d,p)[b]	
CO_2•Benzene					
2.1	C_1	3.02	2.92	2.95	2.78
2.2	C_s	3.01	2.91	2.51	2.77
2.3	C_{2v}	2.87	2.72	2.31	2.56
2.4	C_{6v}	0.46	0.71	0.28	0.82
CO_2•Pyridine					
2.5	C_1	2.69	2.42	2.07	2.36
2.6	C_s	1.02	1.00	0.14	1.01
2.7	C_1	2.33	2.31	1.58	2.31
2.8	C_s	0.67	0.87	0.46	1.05
CO_2•1,3,5-triazine					
2.9	C_1	1.75	1.79	1.83	2.13
2.10	C_s	1.16	1.19	0.48	1.42
2.11	C_{3v}	1.13	1.31	1.69	1.74
MAD[c]		0.29	0.16	0.45	
M%AD		17.9	9.7	32.8	

[a]See main text for structures. [b]Includes counterpoise corrections

Table S6. B971/6-31G(d)-DCP optimized coordinates (Å) for C_1-symmetry C_6H_6•CO_2 dimer.

C	-2.15576500	0.56875000	0.07457000
O	-2.14980700	-0.38163700	-0.61007600
O	-2.19119500	1.52245600	0.75681300
C	0.96661300	-1.38500000	0.85346000
C	0.95684300	-0.05728400	1.32395200
C	1.12880900	1.01134200	0.42074300
C	1.30836400	0.75068000	-0.95210000
C	1.31862700	-0.57774300	-1.42165000
C	1.14819500	-1.64505000	-0.51916700
H	0.83338800	-2.21115000	1.55117600
H	0.81650600	0.14500300	2.38532000
H	1.11820000	2.03804500	0.78447100
H	1.44102200	1.57669200	-1.65020100
H	1.45550700	-0.77899200	-2.48352600
H	1.15216600	-2.67185800	-0.88288800

Table S7. B971/6-31G(d)-DCP optimized coordinates (Å) for C_s-symmetry C_6H_6•CO_2 dimer.

C	-2.16693900	0.65336600	0.00000000
O	-2.21932000	-0.51676300	0.00000000
O	-2.13973300	1.82618400	0.00000000
C	1.13989000	-1.56284500	0.70407300
C	1.13989000	-0.34281900	1.40887000
C	1.14035300	0.87733600	0.70489800
C	1.14035300	0.87733600	-0.70489800
C	1.13989000	-0.34281900	-1.40887000
C	1.13989000	-1.56284500	-0.70407300
H	1.13607300	-2.50638200	1.24865800
H	1.14027200	-0.34300400	2.49844600
H	1.13988500	1.82156500	1.24830800
H	1.13988500	1.82156500	-1.24830800
H	1.14027200	-0.34300400	-2.49844600
H	1.13607300	-2.50638200	-1.24865800

Table S8. B971/6-31G(d)-DCP optimized coordinates (Å) for C_{2v}-symmetry C_6H_6•CO_2 dimer.

C	0.00000000	0.00000000	2.22328400
O	0.00000000	1.17205900	2.23639100
O	0.00000000	-1.17205900	2.23639100
C	-1.22000200	0.70463800	-1.16936800
C	-1.22000200	-0.70463800	-1.16936800
C	0.00000000	-1.40920100	-1.17124600
C	1.22000200	-0.70463800	-1.16936800
C	1.22000200	0.70463800	-1.16936800
C	0.00000000	1.40920100	-1.17124600
H	-2.16337100	1.24967400	-1.16758100
H	-2.16337100	-1.24967400	-1.16758100
H	0.00000000	-2.49837100	-1.16592600
H	2.16337100	-1.24967400	-1.16758100
H	2.16337100	1.24967400	-1.16758100
H	0.00000000	2.49837100	-1.16592600

Table S9. B971/6-31G(d)-DCP optimized coordinates (Å) for C_{6v}-symmetry C_6H_6•CO_2 dimer.

C	0.00000000	1.40846500	-1.55207600
C	1.21976700	0.70423300	-1.55207600
C	1.21976700	-0.70423300	-1.55207600
C	0.00000000	-1.40846500	-1.55207600
C	-1.21976700	-0.70423300	-1.55207600
C	-1.21976700	0.70423300	-1.55207600
H	0.00000000	2.49809200	-1.55275500
H	2.16341100	1.24904600	-1.55275500
H	2.16341100	-1.24904600	-1.55275500
H	0.00000000	-2.49809200	-1.55275500
H	-2.16341100	-1.24904600	-1.55275500
H	-2.16341100	1.24904600	-1.55275500
O	0.00000000	0.00000000	1.79103300
C	0.00000000	0.00000000	2.96245000
O	0.00000000	0.00000000	4.13603500

Table S10. B971/6-31G(d)-DCP optimized coordinates (Å) for C_1-symmetry C_5NH_5•CO_2 dimer.

C	0.02442500	-0.05966400	0.02218200
O	0.02303000	0.34496000	1.11240300
O	0.03856600	-0.46317900	-1.07036600
C	-3.42667000	-0.97239200	0.80659800
C	-3.30669800	-0.29505300	-0.41693500
C	-3.22548700	1.10461000	-0.39866600
C	-3.26397700	1.75990900	0.83902200
C	-3.38615100	0.98422000	2.00236800
H	-3.49409600	-2.05719700	0.82955500
H	-3.27648500	-0.84860400	-1.34881300
H	-3.13432100	1.66676100	-1.32258900
H	-3.20346600	2.84057200	0.90635800
H	-3.41871200	1.45982400	2.97899000
N	-3.46835700	-0.35469200	1.99710900

Table S11. B971/6-31G(d)-DCP optimized coordinates (Å) for C_s-symmetry C_5NH_5•CO_2 dimer.

C	2.25454600	-0.02818200	0.00000000
O	2.25454600	-1.20033000	0.00000000
O	2.25454600	1.14396700	0.00000000
C	-1.18095300	1.38948000	0.00000000
C	-1.18095300	0.68191900	1.22993100
C	-1.18095300	0.68191900	-1.22993100
C	-1.18095300	-0.70225200	1.16752400
C	-1.18095300	-0.70225200	-1.16752400
N	-1.18095300	-1.39256000	0.00000000
H	-1.18095300	2.47896900	0.00000000
H	-1.18095300	1.21148400	2.18088700
H	-1.18095300	1.21148400	-2.18088700
H	-1.18095300	-1.31345400	2.07138200
H	-1.18095300	-1.31345400	-2.07138200

Table S12. B971/6-31G(d)-DCP optimized coordinates (Å) for C_1-symmetry C_5NH_5•CO_2 dimer.

C	2.24904200	0.01151800	0.01095100
O	2.26449000	-1.15834000	-0.06057400
O	2.23462900	1.18138800	0.08249300
C	-1.20569800	0.60606800	1.22819600
C	-1.18773500	-0.80401500	1.14410100
C	-1.19535500	1.38838800	0.04120600
C	-1.16009600	-1.37171200	-0.12756500
C	-1.16750100	0.71405800	-1.16735400
N	-1.15001500	-0.62865200	-1.27119100
H	-1.22827200	1.09676700	2.20091400
H	-1.19580300	-1.42034200	2.04110100
H	-1.20987700	2.47577100	0.08502600
H	-1.14540200	-2.45387200	-0.26486700
H	-1.15943400	1.25201300	-2.11639400

Table S13. B971/6-31G(d)-DCP optimized coordinates (Å) for C_s-symmetry C_5NH_5•CO_2 dimer.

N	1.43040895	-1.52615510	0.00000000
C	0.72822434	-1.53049806	1.14968524
C	-0.67770269	-1.53920699	1.20857751
C	-1.39599705	-1.54366406	0.00000000
C	-0.67770269	-1.53920699	-1.20857751
C	0.72822434	-1.53049806	-1.14968524
H	1.31921786	-1.52683025	2.06735854
H	-1.19042119	-1.54237612	2.16926324
H	-2.48562905	-1.55041404	0.00000000
H	-1.19042119	-1.54237612	-2.16926324
H	1.31921786	-1.52683025	-2.06735854
O	0.00547199	1.75808092	0.00000000
C	-0.00178999	2.93047492	0.00000000
O	-0.00905297	4.10286792	0.00000000

Table S14. B971/6-31G(d)-DCP optimized coordinates (Å) for C_1-symmetry $C_3N_3H_3$•CO_2 dimer.

C	3.02285900	-0.79713000	-0.16369600
C	3.05174800	-3.04722900	-0.26070200
C	4.95201500	-1.91414200	0.17034100
N	2.32137000	-1.92471300	-0.36633600
N	4.33746000	-0.72022800	0.10797200
N	4.36820600	-3.11359500	0.00462400
H	2.52859900	-3.99301400	-0.40484000
H	6.02179800	-1.90950400	0.38192300
H	2.47548300	0.14383300	-0.22635800
C	4.15362200	-2.02801500	3.38884500
O	5.30300400	-2.02404400	3.61823700
O	3.00390400	-2.03202200	3.15939800

Table S15. B971/6-31G(d)-DCP optimized coordinates (Å) for C_s-symmetry $C_3N_3H_3$•CO_2 dimer.

C	2.28604200	0.00019300	0.00000000
O	2.28604200	-1.17202000	0.00000000
O	2.28604200	1.17240500	0.00000000

C	-1.19755600	1.30141500	0.00000000
N	-1.19751800	0.69155700	1.19815500
N	-1.19751800	0.69155700	-1.19815500
C	-1.19755600	-0.65091700	1.12660400
C	-1.19755600	-0.65091700	-1.12660400
N	-1.19751800	-1.38312300	0.00000000
H	-1.19439100	2.39158000	0.00000000
H	-1.19732300	-1.19662300	2.07070000
H	-1.19732300	-1.19662300	-2.07070000

Table S16. B971/6-31G(d)-DCP optimized coordinates (Å) for C_{3v}-symmetry $C_3N_3H_3$•CO_2 dimer.

N	1.49014200	-1.36534600	0.21734100
C	1.56741500	-0.69022700	-0.94176600
N	1.56479200	0.64597300	-1.08247900
C	1.46887100	1.31438900	0.07905000
N	1.38452900	0.76748900	1.30341300
C	1.39921600	-0.57605800	1.30083600
H	1.64172300	-1.28280700	-1.85434700
H	1.46069100	2.40354200	0.02298200
H	1.33382100	-1.07252600	2.26969200
O	-1.65897100	-0.01740500	-0.14854100
C	-2.82408200	-0.03060700	-0.27885800
O	-3.98865300	-0.04384700	-0.40918700

Table S17. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the exterior wall of [6,6]-SWNT.

C	-5.99867800	-4.60484600	0.66310100
C	-1.05497900	-4.30445300	0.69046400
C	-2.31176100	-4.15608900	1.38987500
C	-3.55424600	-4.39698000	0.69841700
C	-4.82137400	-3.58597600	2.66948600
C	-4.79600300	-4.30174800	1.40615700
C	-6.05138700	-3.12516600	3.27433800
C	3.92419500	-4.12972000	0.69877200
C	2.66752800	-3.97805100	1.39015100
C	1.42467700	-4.21596900	0.69066300
C	0.15333200	-3.37737100	2.64769300
C	0.17871600	-4.08956100	1.39146700
C	-1.10498700	-2.90738100	3.15331400
C	-2.33675600	-3.45384600	2.62888600
C	-3.64871800	-1.75613300	3.88294100
C	-3.60392400	-3.00557500	3.15176600
C	-4.90999400	-1.11814400	4.11453500
C	-6.09406800	-1.93532600	3.97074300
C	6.37723000	-4.16233800	0.66378300
C	5.13018000	-3.22954900	2.66962600
C	5.15585600	-3.94621400	1.40649200
C	3.87435000	-2.73756900	3.15173900
C	2.64246700	-3.27562400	2.62902200
C	1.33055900	-1.58299200	3.87629000
C	1.37469800	-2.81872600	3.15337400
C	0.06590700	-0.93525400	4.07770000
C	-1.14919200	-1.67184600	3.87629900
C	-2.47559100	0.40882300	4.06725100

C	-2.42428500	-1.01441100	4.05737900
C	-3.75028100	1.06296600	3.90154700
C	-4.96239000	0.33294100	4.12352100
C	-6.24494100	2.26270100	3.30568700
C	-6.20232000	1.06424700	3.98714000
C	6.28169400	-1.49045100	3.96867200
C	6.32414900	-2.68069200	3.27276900
C	5.04198400	-0.76084100	4.11363400
C	3.82979300	-1.48781600	3.88229100
C	2.50403100	0.58732300	4.06632800
C	2.55520300	-0.83586300	4.05690000
C	1.22893100	1.24713300	3.89527000
C	0.01405200	0.50789700	4.08759100
C	-1.29537900	2.40268000	3.18837400
C	-1.25091500	1.15823400	3.89567600
C	-2.56353500	2.86560700	2.67003200
C	-3.79520000	2.32171200	3.18648400
C	-5.07657100	3.55104800	1.45509500
C	-5.05089100	2.81912200	2.70927200
C	-6.29800100	3.77836600	0.71550300
C	6.17368000	1.50921300	3.98864600
C	4.98972700	0.69045900	4.12319500
C	3.68313600	2.58992900	3.18533700
C	3.72840400	1.33131200	3.90049500
C	2.41555800	3.04465400	2.66891800
C	1.18440300	2.49195300	3.18806400
C	-0.09969900	3.69311300	1.44057100
C	-0.07411900	2.96758400	2.68904300
C	-1.34625300	3.82416400	0.74196600
C	-2.58933700	3.58085300	1.43868000
C	-3.84547000	3.75069500	-0.69830800
C	-3.84527200	3.74194300	0.74927800
C	-5.07696000	3.56927200	-1.40632000
C	-6.29817600	3.78722600	-0.66359000
C	6.13050000	2.70792200	3.30742500
C	4.87373200	3.90880300	1.45559400
C	4.90010400	3.17657600	2.70969400
C	3.63172000	4.01241200	0.74971500
C	2.38966600	3.76191700	1.43860500
C	1.13257800	3.92640400	-0.69006400
C	-0.10013500	3.71031600	-1.39132400
C	-2.56438000	2.89822200	-2.63015600
C	-2.58977300	3.59824700	-1.39000300
C	-3.79625400	2.36114900	-3.15313900
C	-5.05173500	2.85275200	-2.66943700
C	-6.20360200	1.11398100	-3.96879000
C	-6.24597700	2.30386000	-3.27240600
C	6.07563100	4.23078900	-0.66317200
C	6.07593100	4.22197500	0.71616200
C	4.87311800	3.92711500	-1.40603700
C	3.63138800	4.02168800	-0.69834700
C	2.41444100	3.07773600	-2.62877900
C	2.38900300	3.78024800	-1.38984400
C	1.18325200	2.53133400	-3.15431600
C	-0.07511600	3.00008000	-2.64846400
C	-1.25223500	1.20649000	-3.87780200
C	-1.29649600	2.44194000	-3.15480600

C	-2.47699100	0.45943600	-4.05846100
C	-3.75157900	1.11143500	-3.88392900
C	-4.91145300	-1.06670900	-4.12425600
C	-4.96379200	0.38437700	-4.11475400
C	-6.09550900	-1.88557600	-3.99016500
C	6.12914800	2.74946000	-3.27318700
C	4.89896600	3.21052400	-2.66913700
C	3.72693500	1.37998100	-3.88211600
C	3.68182500	2.62969400	-3.15145900
C	2.50261600	0.63803600	-4.05697300
C	1.22757300	1.29547700	-3.87704500
C	0.06451200	-0.88442000	-4.08704700
C	0.01263800	0.55874100	-4.07845900
C	-1.15053000	-1.62351100	-3.89453000
C	-2.42569900	-0.96381800	-4.06683000
C	-3.60505200	-2.96606300	-3.18562000
C	-3.65010000	-1.70763700	-3.90119900
C	-4.82232600	-3.55238300	-2.71011500
C	-6.05256500	-3.08399000	-3.30862400
C	6.17214400	1.55922200	-3.96911400
C	5.04058200	-0.70920500	-4.12213100
C	4.98823600	0.74208200	-4.11329600
C	3.82850200	-1.43920400	-3.89972400
C	2.55383100	-0.78517800	-4.06576800
C	1.37363100	-2.77921800	-3.18668900
C	1.32925900	-1.53460900	-3.89421500
C	0.15241600	-3.34407400	-2.68752800
C	-1.10608700	-2.86793500	-3.18691700
C	-2.31224500	-4.13829500	-1.43858000
C	-2.33768500	-3.42077900	-2.66879800
C	-3.55448600	-4.38782800	-0.74975900
C	-4.79649000	-4.28380000	-1.45579300
C	-5.99890900	-4.59619400	-0.71617900
C	6.32308000	-2.63936000	-3.30570200
C	6.28040100	-1.44049400	-3.98659200
C	5.12929100	-3.19580800	-2.70916800
C	3.87330400	-2.69798200	-3.18481800
C	2.66706700	-3.96020400	-1.43832700
C	2.64158200	-3.24248700	-2.66839500
C	1.42443800	-4.20690200	-0.74149100
C	0.17824200	-4.07175100	-1.44021100
C	-1.05522100	-4.29539500	-0.74155300
C	6.37700200	-4.15360200	-0.71552200
C	5.15539100	-3.92812100	-1.45504500
C	3.92395300	-4.12051000	-0.74932600
H	-7.13675800	0.66811600	-4.30706100
H	-7.21144400	2.76680300	-3.07862700
H	-7.24874800	3.84340900	-1.19014000
H	-7.24845500	3.82780000	1.24293300
H	-7.21048100	2.72797200	3.11795400
H	-7.13534800	0.61407800	4.32001400
H	-7.05624700	-1.55836500	4.31149500
H	-6.98098900	-3.65734900	3.08285700
H	-6.94325600	-4.72680000	1.18928400
H	-6.94365900	-4.71153600	-1.24356000
H	-6.98209600	-3.61848100	-3.12332700
H	-7.05784600	-1.50440600	-4.32574000

H	7.02061800	4.33787800	1.24351700
H	7.02010700	4.35335500	-1.18938700
H	7.05873800	3.28151500	-3.08134400
H	7.13458900	1.18209500	-4.30893700
H	7.21338300	-0.99030800	-4.31956400
H	7.28869100	-3.10478500	-3.11865500
H	7.32771900	-4.20051100	-1.24272700
H	7.32812400	-4.21581500	1.19004900
H	7.28967700	-3.14381400	3.07966500
H	7.21477500	-1.04461100	4.30716600
H	7.13624400	1.12787500	4.32337500
H	7.06006000	3.24218900	3.12168900
C	1.13283300	3.91847100	0.74174300
C	-1.34639600	3.83161500	-0.69042300
C	-1.44791900	6.97778500	-0.00232200
O	-0.27718800	7.03348100	-0.02306400
O	-2.61955600	6.94190200	0.01986400

Table S18. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the interior wall of [6,6]-SWNT.

C	6.08619200	1.17549600	-4.22931700
C	1.14053700	1.18657400	-3.97629300
C	2.39765900	1.85604200	-3.72810200
C	3.64030400	1.19510500	-4.04190200
C	4.90498400	3.04392500	-2.97821900
C	4.88300600	1.87978000	-3.84624400
C	6.13137600	3.58258200	-2.43412200
C	-3.84115700	1.19672400	-3.85691400
C	-2.58413200	1.85762400	-3.60591900
C	-1.34079600	1.18742000	-3.91545300
C	-0.07156600	3.01765500	-2.82540700
C	-0.09355900	1.86024200	-3.68848300
C	1.18296900	3.45677700	-2.28412800
C	2.41893100	2.99736500	-2.87716500
C	3.71540300	4.03168200	-1.02740600
C	3.68260100	3.45643600	-2.35565300
C	4.97018100	4.17974900	-0.35276700
C	6.16284000	4.13050600	-1.16879900
C	-6.29333700	1.17751700	-3.92216800
C	-5.05096300	3.04584200	-2.73182500
C	-5.07242600	1.88186500	-3.60010500
C	-3.79917100	3.45848400	-2.17080900
C	-2.56271700	2.99929900	-2.75479900
C	-1.26534800	4.02591600	-0.90921400
C	-1.29814400	3.45739100	-2.22316700
C	-0.00690900	4.14152800	-0.22821300
C	1.21551700	4.02563600	-0.97084800
C	2.51850300	3.95252100	1.13057700
C	2.48330700	4.11985600	-0.28278300
C	3.78539700	3.69981700	1.77124900
C	5.00617800	4.00839700	1.08888200
C	6.26526200	2.94932700	2.91337600
C	6.23724200	3.77724400	1.81065600
C	-6.21737700	4.12869200	-0.86004800
C	-6.24879400	3.58339100	-2.12631400
C	-4.98569700	4.17769000	-0.10444300

C	-3.76619100	4.03210800	-0.84152200
C	-2.46298400	3.94987400	1.25410400
C	-2.49834100	4.11969900	-0.15926400
C	-1.19534800	3.69009100	1.89933800
C	0.02893200	3.97122500	1.20512400
C	1.31455000	2.83333700	2.98291000
C	1.28566300	3.69395100	1.83952300
C	2.57551600	2.25501200	3.38932900
C	3.81480200	2.83017100	2.92818400
C	5.07868200	0.95582200	3.94677600
C	5.06401400	2.29125800	3.37611600
C	6.29517700	0.18804900	4.09319900
C	-6.14270400	3.77213300	2.11939800
C	-4.94947900	4.00453600	1.33702200
C	-3.66664700	2.82737400	3.11524800
C	-3.69607900	3.69661400	1.95771000
C	-2.40570500	2.25222400	3.51384700
C	-1.16652100	2.82935700	3.04275300
C	0.10008200	0.94311300	4.03176000
C	0.08596300	2.27090200	3.46559000
C	1.34304400	0.22828900	4.09205500
C	2.59000800	0.94554500	3.94779400
C	3.83907000	-1.20141100	3.86334200
C	3.84307700	0.23664700	4.03598200
C	5.07077300	-1.88627800	3.60640400
C	6.29145700	-1.18157300	3.92900200
C	-6.11499300	2.94477700	3.22256800
C	-4.87691200	0.95290000	4.19785100
C	-4.89158900	2.28777400	3.62545400
C	-3.63800200	0.23413300	4.22555000
C	-2.39131700	0.94349000	4.07414600
C	-1.14214400	-1.19432500	3.98553300
C	0.09177300	-1.86745400	3.69678900
C	2.56085800	-3.00490200	2.76211100
C	2.58231400	-1.86299900	3.61238200
C	3.79698600	-3.46389800	2.17790200
C	5.04899600	-3.05063600	2.73818900
C	6.21490100	-4.13518200	0.86674900
C	6.24691500	-3.58830000	2.13255100
C	-6.08782400	-1.18479900	4.24281800
C	-6.08430600	0.18486700	4.40601000
C	-4.88463500	-1.88896000	3.85928400
C	-3.64188200	-1.20390400	4.05355500
C	-2.42036700	-3.00583600	2.88839800
C	-2.39902500	-1.86443700	3.73885400
C	-1.18469500	-3.46525500	2.29551700
C	0.06984200	-3.02541300	2.83506400
C	1.26300100	-4.03198800	0.91848200
C	1.29617400	-3.46342600	2.23186600
C	2.49539800	-4.12661300	0.16782600
C	3.76354500	-4.03875300	0.84935700
C	4.94603100	-4.01415400	-1.32969000
C	4.98270400	-4.18542200	0.11198500
C	6.13912300	-3.78285300	-2.11278400
C	-6.13325000	-3.59033800	2.44663700
C	-4.90651100	-3.05272500	2.99080400
C	-3.71802000	-4.03796500	1.03894900

C	-3.68436600	-3.46446600	2.36760900
C	-2.48607600	-4.12556700	0.29438200
C	-1.21794600	-4.03293300	0.98207200
C	-0.03213300	-3.97573800	-1.19432300
C	0.00412400	-4.14745200	0.23881400
C	1.19187600	-3.69742100	-1.89060500
C	2.45969000	-3.95810100	-1.24568000
C	3.66356100	-2.83669400	-3.10787200
C	3.69260400	-3.70599100	-1.95025500
C	4.88849800	-2.29703900	-3.61737800
C	6.11140600	-2.95508300	-3.21544700
C	-6.16529000	-4.13622500	1.18052500
C	-5.00941300	-4.01147400	-1.07706100
C	-4.97292400	-4.18452700	0.36436200
C	-3.78885500	-3.70262900	-1.75965600
C	-2.52210300	-3.95562500	-1.11863200
C	-1.31818800	-2.83658800	-2.97182800
C	-1.28924400	-3.69603300	-1.82734900
C	-0.08897700	-2.27720500	-3.45742300
C	1.16322700	-2.83780000	-3.03536600
C	2.38903200	-0.95168700	-4.06601100
C	2.40281500	-2.26102200	-3.50668300
C	3.63601400	-0.24258300	-4.21538300
C	4.87438400	-0.96156900	-4.18765100
C	6.08206700	-0.19397600	-4.39378400
C	-6.26848300	-2.95163800	-2.90136700
C	-6.24058100	-3.77954400	-1.79867600
C	-5.06728500	-2.29426600	-3.36502900
C	-3.81836900	-2.83342500	-2.91712700
C	-2.59307200	-0.95038900	-3.94038700
C	-2.57925900	-2.25889100	-3.37957100
C	-1.34552400	-0.23435300	-4.08570400
C	-0.10276600	-0.94971300	-4.02510400
C	1.13589500	-0.23490600	-4.14768500
C	-6.29744000	-0.19208900	-4.08476000
C	-5.08131700	-0.95977600	-3.93743900
C	-3.84574000	-0.24127700	-4.02838600
H	7.15163400	-4.42127200	0.39290000
H	7.20795700	-3.45755900	2.62584900
H	7.23999000	-1.71481700	3.92911200
H	7.24667000	0.70064000	4.21885500
H	7.22508800	2.70176800	3.36212300
H	7.17569100	4.16214000	1.41690300
H	7.12188600	4.41884800	-0.74337100
H	7.06642100	3.45258500	-2.97515300
H	7.03346600	1.70887900	-4.27544400
H	7.02628900	-0.70618400	-4.56622400
H	7.04755100	-2.70765600	-3.71164600
H	7.09629100	-4.16774300	-1.76720200
H	-7.02846300	0.69715600	4.57916500
H	-7.03485200	-1.71843200	4.29082800
H	-7.06792400	-3.46035200	2.98827000
H	-7.12454900	-4.42325900	0.75485100
H	-7.17908900	-4.16415200	-1.40489400
H	-7.22848600	-2.70406600	-3.34945500
H	-7.24908100	-0.70448500	-4.20904000
H	-7.24148700	1.71120900	-3.92229800

H	-7.20959400	3.45412800	-2.62021800
H	-7.15424200	4.41489900	-0.38656200
H	-7.10008100	4.15566600	1.77300000
H	-7.05101400	2.69605900	3.71852800
C	-1.13791800	0.22720300	4.15544900
C	1.33877100	-1.19343000	3.92221800
C	0.01441000	0.06277200	0.31198600
O	-0.97821500	-0.56173400	0.30605300
O	1.00784900	0.68546800	0.31611000

Table S19. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the exterior wall of [6,6]-N-SWNT.

C	6.07978000	1.19804500	-4.30858200
C	1.13957900	1.19543300	-4.01952800
C	2.39341300	1.86788500	-3.78007200
C	3.63802400	1.20884300	-4.09973100
C	4.90509100	3.06172500	-3.04368300
C	4.87933200	1.89837100	-3.91929900
C	6.13126500	3.59107000	-2.50108700
C	-3.84187900	1.19169600	-3.86887600
C	-2.58540500	1.85503300	-3.62041800
C	-1.34256400	1.19016000	-3.94090200
C	-0.07071200	3.01992300	-2.85305500
C	-0.09576800	1.86565000	-3.71893500
C	1.18612700	3.46438800	-2.32526000
C	2.41770100	3.00912200	-2.92589600
C	3.72918700	4.02483000	-1.07387300
C	3.68622000	3.46431400	-2.40757600
C	4.98671500	4.16655300	-0.40520800
C	6.17084500	4.12326500	-1.22565700
C	-6.29227500	1.16771500	-3.92981600
C	-5.05366100	3.02070800	-2.71182400
C	-5.07523500	1.87072200	-3.60186700
C	-3.79947200	3.43242300	-2.15645700
C	-2.56363200	2.98939500	-2.75819000
C	-1.25758000	4.00642100	-0.91991300
C	-1.29840600	3.45118800	-2.23615900
C	0.00922300	4.13030500	-0.25281200
C	1.22849200	4.02902600	-1.00464700
C	2.54100700	3.93486900	1.09034300
C	2.49683300	4.11476600	-0.32370700
C	3.81060000	3.66925300	1.72604800
C	5.03164700	3.97741400	1.04280900
C	6.28200200	2.90776000	2.87189000
C	6.25650500	3.72812400	1.75453000
C	-6.20981800	4.06341200	-0.80953500
C	-6.24868700	3.53572300	-2.08483100
C	-4.97228000	4.12206000	-0.06769400
C	-3.75935200	3.99067800	-0.82095500
C	-2.43685000	3.90582700	1.25550400
C	-2.48506600	4.08682900	-0.15429900
C	-1.16094900	3.64767100	1.88260000
C	0.05897500	3.94616700	1.17520400
C	1.34916400	2.79926200	2.93908100
C	1.31311300	3.67868600	1.80003200
C	2.59563900	2.23030200	3.34338000

C	3.84182300	2.80391900	2.88464100
C	5.08217200	0.94829900	3.97044700
C	5.08275500	2.27753800	3.35337200
C	6.29384200	0.17743000	4.14158600
C	-6.09961900	3.73542300	2.18199000
C	-4.91997200	3.95240000	1.37617500
C	-3.61032900	2.80222000	3.15596300
C	-3.65580900	3.65183800	1.98171700
C	-2.34215600	2.22086000	3.53140500
C	-1.11838200	2.78495200	3.00645400
C	0.14589200	0.91598400	4.01569800
C	0.13117800	2.22351700	3.42122000
C	1.36260400	0.21972200	4.06936100
C	2.59712000	0.92428300	3.90921000
C	3.83915400	-1.20852700	3.92289700
C	3.85732000	0.23476400	4.05859100
C	5.06585800	-1.89828700	3.65982500
C	6.28472800	-1.19314000	3.99303600
C	-6.05303300	2.93501900	3.30618300
C	-4.78665400	0.96487000	4.29841900
C	-4.82381400	2.29149700	3.70731900
C	-3.55134600	0.24217400	4.32051100
C	-2.31043600	0.94119700	4.12461800
C	-1.07948700	-1.16190400	3.97410500
C	0.12818100	-1.81504200	3.68513700
C	2.57158100	-2.95866600	2.76740800
C	2.58270600	-1.84964000	3.64107300
C	3.81113200	-3.42807200	2.19320400
C	5.05885100	-3.05106600	2.77519400
C	6.23178000	-4.09351000	0.88368000
C	6.25736400	-3.57479500	2.16327000
C	-5.99760900	-1.17460700	4.35323800
C	-5.98862900	0.19238600	4.52884000
C	-4.80298200	-1.87414900	3.93328100
C	-3.57090700	-1.19246600	4.11292200
C	-2.36823700	-2.95581300	2.87563300
C	-2.32681500	-1.81694400	3.72814500
C	-1.15178300	-3.40738700	2.27721500
C	0.09704400	-2.95157200	2.80571500
C	1.28489300	-3.97459600	0.90640900
C	1.31555600	-3.39355100	2.19953400
C	2.51930800	-4.07106500	0.16203200
C	3.78096300	-3.98339400	0.85399700
C	4.96988100	-3.95589600	-1.32329800
C	5.00486000	-4.12676000	0.12114400
C	6.16143600	-3.71867600	-2.10338200
C	-6.08057100	-3.53119200	2.48149200
C	-4.85028600	-3.02242000	3.02398900
C	-3.68739700	-3.99062500	1.04557100
C	-3.64334500	-3.41705700	2.37254200
C	-2.45977500	-4.09312000	0.29102100
C	-1.18999900	-4.00073200	0.96646700
C	-0.01357400	-3.95440200	-1.20901700
C	0.02307900	-4.10787700	0.22307900
C	1.21230000	-3.67077600	-1.90296300
C	2.48228500	-3.91859200	-1.25164300
C	3.68033500	-2.80835600	-3.12154100

C	3.71545600	-3.66140400	-1.95190000
C	4.90238800	-2.27029600	-3.63925400
C	6.12862000	-2.90922900	-3.22150900
C	-6.12778200	-4.07037700	1.20507900
C	-4.99154600	-3.98674500	-1.06899600
C	-4.94915500	-4.13985900	0.38328800
C	-3.77490500	-3.68562600	-1.75997900
C	-2.50101700	-3.93886200	-1.12605000
C	-1.30661100	-2.83397200	-2.99667300
C	-1.27464000	-3.68901100	-1.84247800
C	-0.07992500	-2.27096200	-3.48088600
C	1.17892800	-2.82525000	-3.05501900
C	2.39308600	-0.94181600	-4.10319800
C	2.41419800	-2.24622700	-3.52966700
C	3.63742300	-0.22973800	-4.26256500
C	4.87964900	-0.94379000	-4.23535600
C	6.08019000	-0.17492300	-4.45937000
C	-6.25436300	-2.95015500	-2.90340800
C	-6.22182900	-3.76275300	-1.78529300
C	-5.05869400	-2.30100500	-3.38047300
C	-3.80718100	-2.83159700	-2.92817800
C	-2.58657300	-0.95176600	-3.96695300
C	-2.56834900	-2.26039700	-3.40152300
C	-1.34422300	-0.23304600	-4.11569700
C	-0.09798000	-0.94661000	-4.05402800
C	1.13824300	-0.22900600	-4.18491400
C	-6.29281900	-0.20224500	-4.10558000
C	-5.07655000	-0.96616200	-3.96211000
C	-3.84317000	-0.24479900	-4.04962600
H	7.17099800	-4.37071000	0.40946100
H	7.21638900	-3.45875500	2.66426800
H	7.22998400	-1.73165800	4.00345800
H	7.24598600	0.68711400	4.27431100
H	7.24514300	2.64491200	3.30465100
H	7.20135300	4.08076200	1.34606900
H	7.13477100	4.39682600	-0.80112800
H	7.06512700	3.45960400	-3.04387900
H	7.02547500	1.73350300	-4.36413100
H	7.02623900	-0.68442200	-4.63093300
H	7.06518000	-2.65650300	-3.71437800
H	7.12301500	-4.08257200	-1.74696500
H	-6.92771300	0.70634600	4.72247400
H	-6.94286900	-1.70942300	4.42028900
H	-7.01421300	-3.38190100	3.02001300
H	-7.09785100	-4.32485500	0.78302300
H	-7.16079500	-4.13354900	-1.37901400
H	-7.21795800	-2.70324400	-3.34444200
H	-7.24391800	-0.71601200	-4.23010000
H	-7.24298100	1.69708700	-3.92135100
H	-7.21446200	3.39814000	-2.56673900
H	-7.14602300	4.32733800	-0.32162500
H	-7.06328300	4.10900600	1.84211100
H	-6.98128500	2.69911700	3.82284300
N	-1.08651800	0.24756000	4.27976700
N	1.37693700	-1.21664400	4.01350800
C	-0.94631100	-0.76973900	7.19101200
O	-2.11478200	-0.83422300	7.25867100

O	0.22334500	-0.70911500	7.13563800

Table S20. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the interior wall of [6,6]-N-SWNT.

C	6.08923800	1.20175500	-4.28086800
C	1.14726700	1.20637500	-4.02043800
C	2.40065800	1.87621500	-3.77301000
C	3.64637100	1.21590600	-4.08541200
C	4.91012400	3.06401600	-3.01863300
C	4.88756800	1.90359300	-3.89818100
C	6.13400100	3.58844000	-2.46621800
C	-3.83538200	1.20557700	-3.89233100
C	-2.57937500	1.86803200	-3.63846600
C	-1.33479900	1.20328000	-3.95284900
C	-0.06666300	3.02937300	-2.85795600
C	-0.08846800	1.87831100	-3.72733000
C	1.18765400	3.46787600	-2.32005000
C	2.42183800	3.01409100	-2.91520900
C	3.72510500	4.01505600	-1.04947400
C	3.68826400	3.46440800	-2.38723700
C	4.97889600	4.15144100	-0.37291300
C	6.16739200	4.11218800	-1.18703300
C	-6.28535100	1.18238600	-3.96395100
C	-5.05128800	3.03290400	-2.73808600
C	-5.06950100	1.88523400	-3.63115100
C	-3.79933400	3.44049900	-2.17492200
C	-2.56086100	2.99956200	-2.77318200
C	-1.26251000	4.00013100	-0.92281300
C	-1.29701700	3.45662000	-2.24364700
C	0.00114200	4.11729000	-0.24919000
C	1.22397800	4.02113300	-0.99514500
C	2.52509800	3.91063400	1.10641300
C	2.48861600	4.10028400	-0.30617600
C	3.79062100	3.64402700	1.74936400
C	5.01564800	3.95482000	1.07450600
C	6.25510200	2.88502900	2.91111300
C	6.23609500	3.70499500	1.79317900
C	-6.21518800	4.06534100	-0.83504800
C	-6.24868000	3.54578100	-2.11388100
C	-4.98127100	4.11739600	-0.08693100
C	-3.76510800	3.98906900	-0.83551000
C	-2.45291600	3.88654900	1.24578500
C	-2.49373100	4.07743600	-0.16273600
C	-1.18079900	3.62309700	1.87684000
C	0.04305700	3.92190900	1.17708100
C	1.32252100	2.77135700	2.94559700
C	1.29340500	3.65159300	1.80765400
C	2.56654900	2.20599300	3.36111900
C	3.81503000	2.77911800	2.90822200
C	5.04942400	0.92865800	4.00929900
C	5.05339800	2.25549900	3.38669100
C	6.26048300	0.15833300	4.18831700
C	-6.11947800	3.72274700	2.15630700
C	-4.93613800	3.93921800	1.35635600
C	-3.63629500	2.78272700	3.13990400
C	-3.67532400	3.63301200	1.96610300

C	-2.37104300	2.20033400	3.52209100
C	-1.14521600	2.75856600	2.99914300
C	0.11100100	0.89360400	4.02254700
C	0.10137700	2.19781800	3.42172800
C	1.32901800	0.19975200	4.09158800
C	2.56434200	0.90333200	3.93459400
C	3.80669100	-1.22841200	3.96424400
C	3.82445600	0.21542900	4.09529900
C	5.03427400	-1.91773900	3.70464700
C	6.25199000	-1.21241000	4.04215500
C	-6.07909900	2.92139000	3.28041400
C	-4.82041800	0.95199500	4.28435700
C	-4.85317100	2.27661300	3.68809800
C	-3.58594600	0.22741200	4.31559000
C	-2.34219600	0.92255600	4.12079700
C	-1.11413400	-1.18133000	3.99409100
C	0.09399500	-1.83623400	3.71321600
C	2.54300000	-2.97291400	2.79852600
C	2.55100300	-1.86949500	3.67812100
C	3.78483800	-3.43969500	2.22651100
C	5.03032400	-3.06743400	2.81614800
C	6.21082400	-4.09899200	0.92352600
C	6.23113500	-3.58877200	2.20660000
C	-6.03415500	-1.18572800	4.33932400
C	-6.02431500	0.18194900	4.51165800
C	-4.83840500	-1.88784600	3.92785200
C	-3.60587800	-1.20792700	4.11400600
C	-2.39768700	-2.97021200	2.88393500
C	-2.35985900	-1.83535700	3.74015600
C	-1.17897600	-3.41825000	2.28950000
C	0.06704200	-2.96578400	2.82663700
C	1.26421600	-3.97215100	0.92475300
C	1.28858100	-3.40281400	2.22246100
C	2.50191300	-4.06519300	0.18523800
C	3.76048200	-3.98507300	0.88332900
C	4.95947500	-3.94765400	-1.28869100
C	4.98745500	-4.12555200	0.15507600
C	6.15479200	-3.71133600	-2.06306700
C	-6.10895500	-3.53899300	2.46417000
C	-4.88130200	-3.03386200	3.01595600
C	-3.70849000	-3.98803700	1.03817600
C	-3.67076500	-3.42543300	2.36970900
C	-2.47693300	-4.08414400	0.29001600
C	-1.21100500	-3.99821400	0.97301500
C	-0.02379600	-3.93532300	-1.19558600
C	0.00525200	-4.09893600	0.23495900
C	1.20541100	-3.65202900	-1.88315500
C	2.47190800	-3.90463600	-1.22733700
C	3.67968100	-2.79615900	-3.09183200
C	3.70839900	-3.64861600	-1.92180700
C	4.90483700	-2.26214900	-3.60610100
C	6.12810600	-2.90210100	-3.18158500
C	-6.14962400	-4.06942400	1.18393900
C	-5.00152800	-3.97086600	-1.08345100
C	-4.96670300	-4.13272200	0.36808300
C	-3.78125100	-3.66649000	-1.76630000
C	-2.51100200	-3.92049900	-1.12583000

C	-1.30672100	-2.81397400	-2.98898400
C	-1.28125900	-3.66773200	-1.83436300
C	-0.07735400	-2.25379600	-3.46924500
C	1.17853300	-2.80765100	-3.03535600
C	2.39911200	-0.93183300	-4.08720000
C	2.41642200	-2.23275700	-3.50676400
C	3.64525000	-0.22277900	-4.24411800
C	4.88645400	-0.93815700	-4.20779400
C	6.08896400	-0.17150500	-4.42878100
C	-6.25430500	-2.93272400	-2.92433900
C	-6.22771400	-3.74558900	-1.80606000
C	-5.05628000	-2.28448200	-3.39620000
C	-3.80731400	-2.81301600	-2.93481600
C	-2.58058600	-0.93750100	-3.97532500
C	-2.56614100	-2.24271400	-3.40278900
C	-1.33681900	-0.22024100	-4.12149600
C	-0.09135200	-0.93366800	-4.05058800
C	1.14567800	-0.21814000	-4.17971400
C	-6.28580300	-0.18804400	-4.13608100
C	-5.07068900	-0.95201000	-3.98358200
C	-3.83671800	-0.23127800	-4.06829700
H	7.15189100	-4.37447200	0.45199500
H	7.18793800	-3.47690200	2.71277300
H	7.19719400	-1.75094700	4.05681300
H	7.21203600	0.66829300	4.32400200
H	7.21577300	2.62298100	3.34979500
H	7.18330300	4.05795700	1.39052600
H	7.12941700	4.38154400	-0.75554200
H	7.07069400	3.45877600	-3.00455700
H	7.03573600	1.73621500	-4.33251100
H	7.03524900	-0.68245200	-4.59461200
H	7.06728200	-2.65116000	-3.67036100
H	7.11425200	-4.07674400	-1.70252700
H	-6.96401500	0.69754500	4.69783800
H	-6.98084400	-1.71873000	4.40108400
H	-7.04532000	-3.39283500	2.99885300
H	-7.11743800	-4.32129100	0.75515100
H	-7.16896600	-4.11627700	-1.40503000
H	-7.21564200	-2.68570600	-3.37022300
H	-7.23653200	-0.70167700	-4.26387900
H	-7.23575400	1.71237800	-3.96107300
H	-7.21227600	3.41206200	-2.60120600
H	-7.15338000	4.32748400	-0.34999400
H	-7.08116000	4.09767400	1.81236900
H	-7.01035900	2.68669300	3.79221600
N	-1.12188800	0.22874000	4.27973000
N	1.34310300	-1.23854800	4.05236900
C	-0.41423400	-0.01839800	-0.08408800
O	-1.27052200	-0.42564800	0.60653200
O	0.44505900	0.38506000	-0.77068400

Table S21. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the exterior wall of [10,0]-SWNT.

C	6.12189500	-2.15250700	3.45830300
C	6.81305500	-3.12842100	2.68450000
C	4.66481200	-2.15864000	3.46706500

C	3.95083900	-3.12623000	2.68232800
C	1.79252800	-2.15160700	3.46096900
C	2.50929600	-3.12806100	2.68642500
C	0.35404100	-2.15249800	3.46303700
C	-0.36478300	-3.12246600	2.68097500
C	-2.52171900	-2.14527500	3.45314600
C	-1.80281800	-3.12050400	2.67968900
C	-3.96303700	-2.14301900	3.44734500
C	-4.68092000	-3.11020600	2.66742200
C	-6.82133700	-2.16137700	3.48269400
C	-6.13794300	-3.11587800	2.67494400
C	6.12518500	0.25476400	3.95518100
C	6.81603100	-0.99060900	3.90617700
C	4.66734600	0.25737500	3.96517000
C	3.95206700	-0.98738600	3.89987200
C	1.79456000	0.25875600	3.96209900
C	2.51100700	-0.98739400	3.90810800
C	0.35568200	0.26031800	3.96510900
C	-0.36435500	-0.98437500	3.90203600
C	-2.52024000	0.26182300	3.95431100
C	-1.80223300	-0.98292500	3.90104600
C	-3.96174500	0.26275700	3.94740500
C	-4.68214000	-0.97762900	3.88097800
C	-6.82045300	0.26985500	3.99047400
C	-6.13956200	-0.97872700	3.89445300
C	6.12441300	2.49721100	2.94752800
C	6.81757800	1.45829500	3.63564400
C	4.66802800	2.50854700	2.95561100
C	3.95414800	1.45898100	3.63146800
C	1.79621000	2.50250600	2.94964000
C	2.51298600	1.46228800	3.63952100
C	0.35801000	2.50635800	2.95183900
C	-0.36226200	1.46280400	3.63456700
C	-2.51737100	2.50278400	2.94248700
C	-1.80008000	1.46395000	3.63308800
C	-3.95852900	2.50264600	2.93723900
C	-4.67939800	1.46069900	3.61420600
C	-6.81651600	2.53083200	2.96404900
C	-6.13682200	1.46603000	3.62574700
C	6.12260700	3.72142300	0.81394200
C	6.81694200	3.27752000	1.97761900
C	4.66798300	3.73833200	0.81537600
C	3.95590000	3.28108900	1.97711200
C	1.79798600	3.72103900	0.81025300
C	0.36068000	3.72227800	0.81007100
C	-2.51450000	3.71834700	0.80595800
C	-1.79691900	3.28394400	1.97463400
C	-3.95487600	3.71913800	0.80333100
C	-4.67410400	3.27811800	1.96503600
C	-6.81157500	3.75394000	0.80738900
C	-6.13077800	3.28676600	1.96974500
C	6.12579800	3.45137000	-1.63140000
C	6.81790700	3.77646000	-0.42904100
C	4.67068600	3.46691200	-1.63838200
C	3.95756300	3.78270200	-0.43249000
C	1.79986800	3.45318300	-1.63680700
C	2.51611000	3.78421000	-0.43463500

C	0.36253000	3.45431500	-1.63970500
C	-0.35713200	3.77381600	-0.43645300
C	-2.51240500	3.44899300	-1.63900400
C	-1.79532500	3.77688000	-0.43737100
C	-3.95334800	3.44988300	-1.63853300
C	-4.67023000	3.77740800	-0.43954200
C	-6.81004800	3.48353100	-1.65575900
C	-6.12674200	3.78658100	-0.44224700
C	6.13122500	1.79102400	-3.44548000
C	6.82212500	2.76601100	-2.67029200
C	4.67423100	1.79932400	-3.45742500
C	3.95992300	2.76822900	-2.67456600
C	1.80224300	1.79637100	-3.45831600
C	2.51846500	2.77171200	-2.68148200
C	0.36393100	1.79914400	-3.46426700
C	-0.35516700	2.76934300	-2.68294300
C	-2.51204200	1.79660400	-3.45946100
C	-1.79298100	2.76999000	-2.68421800
C	-3.95342600	1.79660500	-3.45572400
C	-4.67122000	2.76481200	-2.67677500
C	-6.81165900	1.81909500	-3.49567600
C	-6.12815100	2.77251800	-2.68667200
C	6.13208700	-0.61631900	-3.94242900
C	6.82465900	0.62800800	-3.89165000
C	4.67431000	-0.61685800	-3.95522900
C	3.96081900	0.62896300	-3.89163800
C	1.80166900	-0.61429100	-3.95784100
C	2.51987100	0.63098800	-3.90319300
C	0.36282100	-0.61390600	-3.96387400
C	-0.35547300	0.63196300	-3.90399600
C	-2.51319700	-0.61068100	-3.95909800
C	-1.79338700	0.63296800	-3.90568600
C	-3.95476400	-0.60928600	-3.95503900
C	-4.67347500	0.63228300	-3.89041900
C	-6.81347000	-0.61212100	-4.00381200
C	-6.13088900	0.63547700	-3.90631700
C	6.12628000	-2.85884200	-2.93508300
C	6.82217800	-1.82084900	-3.62170200
C	4.66984300	-2.86798900	-2.94570400
C	3.95870400	-1.81741600	-3.62278800
C	1.79793100	-2.85809400	-2.94457500
C	2.51753000	-1.81863800	-3.63312400
C	0.35972100	-2.85970700	-2.94896600
C	-0.35746300	-1.81498500	-3.63318900
C	-2.51589400	-2.85085600	-2.94576400
C	-1.79545800	-1.81358300	-3.63509300
C	-3.95708400	-2.84857800	-2.94377500
C	-4.67495000	-1.80589800	-3.62277700
C	-6.81500800	-2.87304400	-2.97723800
C	-6.13239900	-1.80923300	-3.63753900
C	6.11935900	-4.08263000	-0.80143500
C	6.81624500	-3.63995000	-1.96399300
C	4.66469100	-4.09789500	-0.80576800
C	3.95486200	-3.63957000	-1.96857500
C	1.79360300	-4.07884500	-0.80644900
C	2.51315300	-3.64141700	-1.97386100
C	0.35619500	-4.08117400	-0.80862800

C	-0.36048800	-3.63531000	-1.97492600
C	-2.51911100	-4.06814800	-0.80966100
C	-1.79854200	-3.63333600	-1.97651200
C	-3.95988500	-4.06593000	-0.81029700
C	-4.67595500	-3.62313000	-1.97325000
C	-6.81676100	-4.09632900	-0.82039900
C	-6.13270900	-3.62968600	-1.98110600
C	6.11813800	-3.81245800	1.64380100
C	6.81227000	-4.13871100	0.44288100
C	4.66292500	-3.82620900	1.64783900
C	3.95175900	-4.14103700	0.44053000
C	1.79165400	-3.80946900	1.64076500
C	2.50977700	-4.14262700	0.43979800
C	0.35400900	-3.81159800	1.64077100
C	-0.36331800	-4.13567400	0.43642000
C	-2.52133700	-3.79932600	1.63404600
C	-1.80141900	-4.13337800	0.43496900
C	-3.96226000	-3.79698900	1.63092300
C	-4.67804400	-4.12340900	0.43089200
C	-6.81937700	-3.82601200	1.64313500
C	-6.13453500	-4.12994800	0.43069800
H	7.90313200	-3.11247500	2.66766000
H	7.90600600	-0.98734200	3.88306500
H	7.90240700	-4.11471500	0.44071700
H	7.90757200	1.44881000	3.61401300
H	7.90630600	-3.61992700	-1.94904000
H	7.90700000	3.25610300	1.96444500
H	7.91214700	-1.81290700	-3.59811300
H	7.90801500	3.75121600	-0.42475600
H	7.91458500	0.62324200	-3.86649000
H	7.91214500	2.74880900	-2.65130500
H	-7.90009900	3.47062800	-1.64909900
H	-7.91030900	0.26903100	3.97254400
H	-7.90163700	3.73951600	0.80256600
H	-7.90647100	2.52172000	2.95016500
H	-7.91122200	-2.15288800	3.46651200
H	-7.90157800	1.81220700	-3.48128800
H	-7.90939000	-3.81120200	1.63469400
H	-7.90335600	-0.60958100	-3.98786600
H	-7.90497900	-2.86212500	-2.96557300
H	-7.90680100	-4.07987500	-0.81783300
C	2.51427300	3.28417100	1.97964200
C	-0.35908200	3.28210300	1.97621800
C	0.05540100	6.89484900	-0.00825000
O	1.01667400	6.83298000	-0.67588000
O	-0.90600300	6.96983200	0.65846900

Table S22. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the interior wall of [10,0]-SWNT.

C	6.12873100	-2.37156600	3.19692200
C	6.81086800	-3.26707700	2.32239100
C	4.67179100	-2.36431800	3.18696000
C	3.95306300	-3.23416200	2.29950800
C	1.79405800	-2.37097300	3.19774900
C	2.51208700	-3.23812900	2.30342400
C	0.35656900	-2.37034800	3.19753200

C	-0.36140000	-3.24346900	2.30770200
C	-2.51629000	-2.37420200	3.20003500
C	-1.79855900	-3.24190700	2.30524700
C	-3.95767800	-2.37136000	3.19408500
C	-4.66983400	-3.25181500	2.30983700
C	-6.81974700	-2.37313600	3.19497700
C	-6.12572100	-3.24065300	2.30195800
C	6.12978300	-0.04033700	3.98623400
C	6.81171200	-1.27928300	3.80705200
C	4.67276900	-0.04005800	3.97422700
C	3.95391600	-1.26545400	3.76786200
C	1.79437000	-0.03966800	3.98767400
C	2.51295400	-1.26619300	3.77179200
C	0.35665700	-0.03946900	3.98752800
C	-0.36193400	-1.26853500	3.77983300
C	-2.51746700	-0.04029700	3.99083200
C	-1.79968700	-1.26806000	3.77575100
C	-3.95875300	-0.04092800	3.98305700
C	-4.67125500	-1.27256900	3.78347400
C	-6.82135700	-0.04177200	3.98369100
C	-6.12757000	-1.26858300	3.77099500
C	6.12991900	2.30956200	3.25480400
C	6.81244800	1.20226200	3.83793400
C	4.67295400	2.30284900	3.24480600
C	3.95439700	1.19036700	3.79876500
C	1.79437400	2.30995200	3.25543300
C	2.51338600	1.19159500	3.80265800
C	0.35665200	2.30968800	3.25465600
C	-0.36224400	1.19409200	3.81044100
C	-2.51767500	2.31197800	3.25767100
C	-1.80016600	1.19265200	3.80657600
C	-3.95900200	2.30808900	3.25145300
C	-4.67225200	1.19452700	3.81323500
C	-6.82169800	2.30849000	3.25174700
C	-6.12867800	1.19013100	3.79982400
C	6.12955800	3.78120900	1.28195900
C	6.81226200	3.22784500	2.40425700
C	4.67257900	3.77031400	1.27788200
C	3.95434500	3.19491600	2.37944100
C	1.79439200	3.77951800	1.28090100
C	0.35630300	3.78017200	1.28053200
C	-2.51749600	3.78416500	1.28132400
C	-1.80012300	3.19974900	2.38253700
C	-3.95885700	3.77894500	1.27907300
C	-4.67190500	3.20905000	2.38842600
C	-6.82088900	3.77990800	1.27903600
C	-6.12817700	3.19792400	2.38020500
C	6.12950500	3.80937800	-1.17947900
C	6.81221900	4.02137900	0.05377800
C	4.67268000	3.79930300	-1.17622700
C	3.95450900	3.98211800	0.05307000
C	1.79466800	3.81144500	-1.18012400
C	2.51361200	3.98500700	0.05297500
C	0.35681700	3.81220900	-1.18037500
C	-0.36222100	3.99422900	0.05237500
C	-2.51700600	3.81609100	-1.18305100
C	-1.79997500	3.98945200	0.05168700

C	-3.95844400	3.81019800	-1.18118100
C	-4.67135000	4.00191000	0.05138200
C	-6.82054400	3.80937200	-1.18132100
C	-6.12731600	3.98757400	0.05121500
C	6.12935200	2.38759700	-3.18897600
C	6.81220200	3.28295200	-2.31471500
C	4.67240700	2.38104100	-3.17911700
C	3.95441000	3.25140300	-2.29163600
C	1.79462500	2.38964600	-3.18945600
C	2.51354800	3.25485500	-2.29398900
C	0.35712000	2.39045400	-3.18928400
C	-0.36144000	3.26361900	-2.29982400
C	-2.51645400	2.39296000	-3.19467300
C	-1.79914300	3.26026200	-2.29876000
C	-3.95783900	2.38875900	-3.18924000
C	-4.67103000	3.26854700	-2.30498600
C	-6.82006100	2.38851900	-3.19030700
C	-6.12694700	3.25636000	-2.29693800
C	6.12864600	0.05626500	-3.97769400
C	6.81150600	1.29475300	-3.79889800
C	4.67168900	0.05649500	-3.96500600
C	3.95367400	1.28234500	-3.75933800
C	1.79371000	0.05839600	-3.97856300
C	2.51261500	1.28489000	-3.76472000
C	0.35670500	0.05914300	-3.97762100
C	-0.36140300	1.28861400	-3.77165900
C	-2.51559600	0.05838200	-3.98541000
C	-1.79900700	1.28685700	-3.76939400
C	-3.95693100	0.05766800	-3.97623500
C	-4.67045700	1.28909200	-3.77823700
C	-6.81968000	0.05692200	-3.97786900
C	-6.12677700	1.28423700	-3.76574800
C	6.12736700	-2.29325500	-3.24632400
C	6.81068900	-1.18655200	-3.82949300
C	4.67044400	-2.28574300	-3.23579600
C	3.95202800	-1.17353600	-3.79077300
C	1.79317900	-2.29166600	-3.24574700
C	2.51127900	-1.17364400	-3.79425800
C	0.35652100	-2.29064400	-3.24468700
C	-0.36127100	-1.17468200	-3.80037400
C	-2.51476900	-2.29522200	-3.25116200
C	-1.79852200	-1.17418300	-3.79777100
C	-3.95615800	-2.29117100	-3.24338600
C	-4.66972500	-1.17808300	-3.80572400
C	-6.81877600	-2.29284500	-3.24501300
C	-6.12613900	-1.17438000	-3.79304800
C	6.12685100	-3.76475900	-1.27367600
C	6.80964800	-3.21153200	-2.39587700
C	4.66999700	-3.75290700	-1.26916200
C	3.95156000	-3.17843900	-2.37118500
C	1.79307200	-3.76367500	-1.27237900
C	2.51099000	-3.18038700	-2.37286700
C	0.35629900	-3.76289800	-1.27204300
C	-0.36133900	-3.18563300	-2.37698700
C	-2.51457500	-3.76976600	-1.27482900
C	-1.79828100	-3.18333700	-2.37558100
C	-3.95555500	-3.76486000	-1.27268700

C	-4.66890300	-3.19267600	-2.38095500
C	-6.81819100	-3.76486200	-1.27319700
C	-6.12503200	-3.18227400	-2.37367200
C	6.12757300	-3.79304600	1.18731700
C	6.81006600	-4.00518900	-0.04591900
C	4.67078400	-3.78252300	1.18407300
C	3.95169900	-3.96677700	-0.04464500
C	1.79343100	-3.79388800	1.18916500
C	2.51107800	-3.96997500	-0.04405300
C	0.35655200	-3.79306500	1.18897100
C	-0.36127400	-3.97688600	-0.04390300
C	-2.51489700	-3.80089500	1.19011300
C	-1.79806200	-3.97454000	-0.04450900
C	-3.95601300	-3.79609300	1.18781000
C	-4.66885200	-3.98669400	-0.04515900
C	-6.81878400	-3.79449200	1.18658500
C	-6.12471500	-3.97280600	-0.04544400
H	7.90085100	-3.25470800	2.31296200
H	7.90166600	-1.27458300	3.79186200
H	7.90004400	-3.99018300	-0.04614800
H	7.90239600	1.19734700	3.82264300
H	7.89961700	-3.19955600	-2.38665500
H	7.90222100	3.21511900	2.39457700
H	7.90064400	-1.18252700	-3.81474700
H	7.90219200	4.00556000	0.05359400
H	7.90146100	1.28925100	-3.78411300
H	7.90218100	3.26980300	-2.30558000
H	-7.91057800	3.78573400	-1.17411400
H	-7.91135500	-0.04200100	3.95909800
H	-7.91091300	3.75657100	1.27068900
H	-7.91171000	2.29434600	3.23137700
H	-7.90977100	-2.35924700	3.17488700
H	-7.91007700	2.37373300	-3.17070900
H	-7.90883000	-3.77183900	1.17893000
H	-7.90968700	0.05636500	-3.95386500
H	-7.90880900	-2.27952200	-3.22520900
H	-7.90823300	-3.74250200	-1.26539200
C	2.51330600	3.19694800	2.38134500
C	-0.36193600	3.20328600	2.38536300
C	0.06783900	-0.31810000	-0.14285800
O	1.24197500	-0.32779400	-0.21968900
O	-1.10631400	-0.33408200	-0.07777700

Table S23. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the exterior wall of [10,0]-N-SWNT.

C	-6.13023000	0.03080100	-3.86195400
C	-6.82142600	-1.20702800	-3.77182900
C	-4.66786400	0.01928300	-3.89033400
C	-3.95382100	-1.22788500	-3.79865200
C	-1.79504100	0.00157600	-3.92890800
C	-2.51359000	-1.23746500	-3.82491700
C	-0.35417900	0.00265300	-3.93700500
C	0.36930700	-1.23555600	-3.82751600
C	2.51989700	0.02236200	-3.91247800
C	1.80611300	-1.22386900	-3.81851500
C	3.96420300	0.03587700	-3.89156400

C	4.69032500	-1.19363700	-3.77629100
C	6.81962000	0.06209000	-3.93845300
C	6.14739700	-1.18397100	-3.78609400
C	-6.10272800	2.33915400	-2.99623800
C	-6.80831900	1.26021800	-3.60466700
C	-4.64310700	2.32652700	-3.00306500
C	-3.94580000	1.22369800	-3.62612800
C	-1.78641700	2.27575400	-3.00310100
C	-2.51106900	1.21536700	-3.65167300
C	-0.35978600	2.27864500	-3.00747400
C	0.36377500	1.21440900	-3.65545500
C	2.49941500	2.31631600	-3.01241200
C	1.79476100	1.22723200	-3.65050100
C	3.94233400	2.33788800	-3.01030500
C	4.67306000	1.25592900	-3.61881400
C	6.79492200	2.39271300	-3.05226400
C	6.12895800	1.27150300	-3.63542700
C	-6.06579100	3.79382900	-1.00143400
C	-6.76954000	3.23140400	-2.11170600
C	-4.61124600	3.79794400	-1.00693000
C	-3.92479700	3.15947600	-2.10399400
C	-1.77065400	3.67885300	-0.98041000
C	-2.48758700	3.11572600	-2.08287200
C	-0.36840000	3.67757600	-0.98152500
C	0.34649100	3.10877600	-2.08279000
C	2.48149000	3.74361400	-0.99709700
C	1.77951600	3.14765800	-2.11000200
C	3.92212100	3.75289100	-0.99167800
C	4.64330300	3.20430100	-2.11487700
C	6.78238200	3.78704800	-1.00343800
C	6.10270200	3.21873100	-2.12481600
C	-6.06815600	3.65885000	1.43189000
C	-6.76784700	3.95095400	0.22699400
C	-4.61356200	3.66185400	1.44049700
C	-3.89877800	3.92015900	0.22808600
C	-1.77293100	3.54595200	1.40629600
C	-0.37092600	3.54521800	1.41017500
C	2.47926400	3.60934300	1.43798000
C	1.76059100	3.89181200	0.23145900
C	3.92033400	3.61831500	1.43616100
C	4.63956000	3.91825000	0.23576100
C	6.78018400	3.65053500	1.45698900
C	6.09462500	3.91151000	0.23681100
C	-6.10830900	1.99089000	3.25200500
C	-6.77382100	2.97580000	2.47110300
C	-4.64884900	1.97751100	3.26018900
C	-3.92902300	2.90552300	2.46087200
C	-1.79224200	1.92671000	3.26017100
C	-2.49155700	2.86444100	2.43781400
C	-0.36598600	1.92886400	3.26770100
C	0.34176800	2.85719700	2.44244000
C	2.49347000	1.96513700	3.28127800
C	1.77509800	2.89203500	2.47624100
C	3.93654000	1.98653700	3.28425000
C	4.63929900	2.94760200	2.49279700
C	6.78910700	2.03617100	3.33798000
C	6.09876400	2.96063600	2.50694700

C	-6.13755600	-0.39910300	3.85703000
C	-6.81517000	0.85116200	3.73545500
C	-4.67526500	-0.41378300	3.88672300
C	-3.95274800	0.81219200	3.75794500
C	-1.80261200	-0.43598000	3.92877400
C	-2.51812400	0.80086700	3.78507700
C	-0.36178000	-0.43600300	3.93974400
C	0.35659900	0.79919900	3.79418800
C	2.51235800	-0.41403100	3.92285300
C	1.78759500	0.81219700	3.79331700
C	3.95676900	-0.39852000	3.90639100
C	4.66615300	0.84399700	3.77074200
C	6.81213900	-0.37799400	3.96151100
C	6.12193800	0.85749200	3.79186600
C	-6.13140200	-2.71618200	3.03427600
C	-6.82865500	-1.61934400	3.62945700
C	-4.67320100	-2.73513400	3.05439200
C	-3.96104300	-1.64347900	3.65980400
C	-1.79666100	-2.74224200	3.07354100
C	-2.52089600	-1.65612400	3.68770200
C	-0.35657400	-2.74387800	3.08066600
C	0.36201700	-1.65479700	3.69616600
C	2.52335400	-2.71959800	3.07018000
C	1.79884000	-1.64243900	3.69134300
C	3.96570700	-2.70652100	3.06053200
C	4.68315300	-1.60797300	3.65813300
C	6.82412200	-2.71350000	3.09422400
C	6.14033700	-1.59958500	3.67156900
C	-6.11371000	-4.10588500	1.00882200
C	-6.81625200	-3.57306500	2.13185500
C	-4.66013300	-4.12025200	1.01466100
C	-3.95327600	-3.58062000	2.14511100
C	-1.78700500	-4.09377500	1.01659700
C	-2.51015700	-3.58385800	2.15503000
C	-0.34989200	-4.09299500	1.01924300
C	0.36645100	-3.57535000	2.15836700
C	2.52806000	-4.07295100	1.01974100
C	1.80593800	-3.56697100	2.15902200
C	3.96792100	-4.06819800	1.01918600
C	4.68456900	-3.54419600	2.15137800
C	6.82577800	-4.08742000	1.03101800
C	6.14280500	-3.54058200	2.15919100
C	-6.11131900	-3.97079800	-1.44350300
C	-6.80571900	-4.23458800	-0.22879600
C	-4.65769500	-3.98475400	-1.44805400
C	-3.94582600	-4.23330200	-0.22583500
C	-1.78457900	-3.95822100	-1.44104700
C	-2.50248700	-4.22834400	-0.22407500
C	-0.34744200	-3.95730800	-1.44077500
C	0.37027700	-4.21477300	-0.22045000
C	2.53047000	-3.93748800	-1.43325800
C	1.80961700	-4.20920100	-0.21872100
C	3.97038100	-3.93291300	-1.42932400
C	4.68440300	-4.19983000	-0.21531800
C	6.82817700	-3.95065700	-1.43751800
C	6.14244200	-4.19838800	-0.21383300
C	-6.12510800	-2.36324200	-3.30090900

C	-6.81166200	-3.31553000	-2.50144500
C	-4.66695000	-2.38003600	-3.32012600
C	-3.94875200	-3.32220600	-2.50987600
C	-1.79038200	-2.38511500	-3.33398900
C	-2.50554600	-3.32437500	-2.51716800
C	-0.35032200	-2.38607500	-3.33842700
C	0.37102700	-3.31586600	-2.51382400
C	2.52960600	-2.36336400	-3.31962300
C	1.81055500	-3.30752500	-2.51069500
C	3.97191000	-2.35146300	-3.30570100
C	4.68915600	-3.28581100	-2.49469100
C	6.83034200	-2.35493000	-3.33466900
C	6.14746000	-3.28139000	-2.49917500
H	-7.91102700	-1.20221900	-3.73760000
H	-7.89807200	1.26246300	-3.57708400
H	-7.90159700	-3.29778300	-2.47767700
H	-7.85949000	3.23043900	-2.08755300
H	-7.89585100	-4.20937600	-0.22839400
H	-7.85732700	3.93542200	0.22499200
H	-7.90612400	-3.55259500	2.10805300
H	-7.86373600	2.97780000	2.44518100
H	-7.91821700	-1.61063400	3.59456000
H	-7.90486200	0.85674000	3.70599700
H	7.87892700	2.03674700	3.31789100
H	7.88471900	2.39153800	-3.03050200
H	7.87030800	3.63925600	1.45119700
H	7.87248700	3.77463300	-0.99704700
H	7.90915600	0.06865100	-3.91144600
H	7.90172000	-0.36850700	3.93732900
H	7.92004400	-2.34122300	-3.31163300
H	7.91388600	-2.69778400	3.07516100
H	7.91580200	-4.06763000	1.02519100
H	7.91820300	-3.93238400	-1.42748400
N	-2.49276000	3.95361600	0.23150800
N	0.35638500	3.94567200	0.23397900
C	-0.07812200	6.90639200	-0.14841900
O	0.74045000	6.91070100	-0.98778600
O	-0.89852700	6.91331000	0.68894600

Table S24. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the interior wall of [10,0]-N-SWNT.

C	-6.15117500	3.85177400	-0.16765800
C	-6.84511200	3.63457500	-1.38804100
C	-4.68880200	3.87684900	-0.18533000
C	-3.97771600	3.65688300	-1.41792300
C	-1.81682000	3.90926800	-0.21338200
C	-2.53777000	3.68045500	-1.43337300
C	-0.37622300	3.91664900	-0.21593400
C	0.34483300	3.68247400	-1.43725500
C	2.49722800	3.89879000	-0.19991000
C	1.78122600	3.67639000	-1.42772800
C	3.94135000	3.88294400	-0.18726100
C	4.66496200	3.64345100	-1.39994900
C	6.79643900	3.93778800	-0.17226200
C	6.12207200	3.65629400	-1.39446300
C	-6.11868400	3.23829400	2.22065700

C	-6.82639500	3.72664700	1.08360200
C	-4.65911300	3.24207700	2.20410600
C	-3.96433000	3.73994500	1.03827800
C	-1.80290800	3.23387000	2.14650000
C	-2.52987500	3.76223500	1.02374000
C	-0.37664500	3.23809900	2.14601200
C	0.34453000	3.76459500	1.01627500
C	2.48263400	3.25040700	2.17716800
C	1.77511800	3.76307800	1.02655200
C	3.92536300	3.25322300	2.19600200
C	4.65296400	3.74203500	1.05311000
C	6.77784800	3.30553100	2.24009800
C	6.10870800	3.76293100	1.06383600
C	-6.07912500	1.41701600	3.88737900
C	-6.78393100	2.45833000	3.20646800
C	-4.62441000	1.42301600	3.88930800
C	-3.93921900	2.44154700	3.13080400
C	-1.78344000	1.38378600	3.76868400
C	-2.50198700	2.41444000	3.08616400
C	-0.38088500	1.38467600	3.76644000
C	0.33212800	2.41435600	3.07417900
C	2.46949400	1.40910800	3.82297800
C	1.76535400	2.44638900	3.10575000
C	3.91041800	1.40518500	3.82749700
C	4.62920400	2.46108900	3.15538700
C	6.77071600	1.42205600	3.85145800
C	6.08875900	2.47384900	3.16490900
C	-6.08049400	-1.01615500	4.01207200
C	-6.78038400	0.21247700	4.17687100
C	-4.62586400	-1.02405200	4.01482200
C	-3.91139100	0.20883700	4.14421100
C	-1.78478500	-1.00100300	3.89089800
C	-0.38221500	-1.00388600	3.88898900
C	2.46837400	-1.02523700	3.94791300
C	1.74809600	0.20361600	4.10706100
C	3.90930500	-1.02191300	3.95182000
C	4.62917500	0.20326900	4.12293600
C	6.76975400	-1.03837900	3.97728100
C	6.08402700	0.20211300	4.11090600
C	-6.12252800	-2.99848100	2.54111900
C	-6.78676300	-2.12091500	3.44200700
C	-4.66295500	-3.00633900	2.52563800
C	-3.94193600	-2.11623000	3.36553000
C	-1.80640500	-3.00844200	2.46867800
C	-2.50464100	-2.09575900	3.31888200
C	-0.38003700	-3.01472600	2.46902200
C	0.32981400	-2.10037900	3.30732400
C	2.47967700	-3.02621300	2.50082400
C	1.76310700	-2.13050600	3.34204300
C	3.92249600	-3.02768200	2.51914400
C	4.62722500	-2.14174100	3.39199700
C	6.77508900	-3.07654600	2.56721700
C	6.08670800	-2.15438400	3.40231700
C	-6.15548200	-3.84665000	0.22602100
C	-6.83080800	-3.59724300	1.45850900
C	-4.69314600	-3.87545400	0.21142700
C	-3.96862500	-3.62002700	1.41589600

C	-1.82110300	-3.91440600	0.18761800
C	-2.53409200	-3.64603400	1.40430000
C	-0.38054800	-3.92377000	0.18608600
C	0.34058700	-3.65292000	1.39762100
C	2.49329800	-3.90748200	0.19998700
C	1.77143000	-3.65178100	1.40755300
C	3.93748000	-3.89142600	0.21044800
C	4.64952000	-3.62908500	1.43068900
C	6.79246800	-3.94677400	0.23009000
C	6.10535700	-3.64948500	1.44290300
C	-6.15449000	-3.27710100	-2.16646300
C	-6.84892700	-3.75030800	-1.01003100
C	-4.69635700	-3.29715400	-2.18615900
C	-3.98162700	-3.77831300	-1.03657600
C	-1.82060000	-3.31232800	-2.19641100
C	-2.54175600	-3.80465600	-1.04900900
C	-0.38072600	-3.31828600	-2.19963900
C	0.34070800	-3.81000200	-1.05214400
C	2.49905900	-3.30681100	-2.18344600
C	1.77719600	-3.80505400	-1.04360200
C	3.94124600	-3.29760000	-2.17502200
C	4.66095000	-3.77318400	-1.02017900
C	6.79931100	-3.33435000	-2.18515800
C	6.11793400	-3.78722300	-1.01385700
C	-6.14167800	-1.41830300	-3.77215900
C	-6.84207600	-2.47592900	-3.11636900
C	-4.68815700	-1.42472300	-3.78973500
C	-3.97915200	-2.48735000	-3.12920200
C	-1.81528800	-1.42180900	-3.77075700
C	-2.53620300	-2.49598200	-3.13463700
C	-0.37809300	-1.42363600	-3.77251400
C	0.34040900	-2.49629200	-3.13088100
C	2.50046400	-1.42114800	-3.75654500
C	1.77977500	-2.49625000	-3.12524800
C	3.94025100	-1.42046400	-3.75467000
C	4.65819400	-2.48794600	-3.11028600
C	6.79803500	-1.43425400	-3.77745900
C	6.11643700	-2.49573800	-3.10883000
C	-6.14056600	1.03381700	-3.89790400
C	-6.83503600	-0.20195200	-4.03053700
C	-4.68715000	1.03737400	-3.91642100
C	-3.97492200	-0.20338100	-4.03742900
C	-1.81401200	1.03454300	-3.89851800
C	-2.53170600	-0.20384000	-4.03722200
C	-0.37673900	1.03507500	-3.90105400
C	0.34185500	-0.20480100	-4.02930700
C	2.50203200	1.03008900	-3.88338100
C	1.78118800	-0.20560600	-4.02503800
C	3.94175900	1.02725700	-3.88059300
C	4.65612500	-0.20746200	-4.01965800
C	6.79972300	1.03461400	-3.90384900
C	6.11412800	-0.20851200	-4.02016100
C	-6.15146600	3.04722000	-2.49147500
C	-6.84002800	2.15374200	-3.35448700
C	-4.69332200	3.06407000	-2.51366200
C	-3.97698200	2.16175700	-3.36940500
C	-1.81723300	3.07630100	-2.52685300

C	-2.53400900	2.16898700	-3.37658500
C	-0.37718100	3.08069300	-2.53107900
C	0.34318200	2.16754500	-3.37415200
C	2.50266500	3.06640200	-2.51221400
C	1.78251800	2.16563900	-3.36735400
C	3.94483900	3.05592800	-2.50193900
C	4.66111300	2.15406300	-3.34921300
C	6.80317300	3.08729100	-2.51428900
C	6.11930100	2.15987100	-3.34784700
H	-7.93474800	3.60238600	-1.37757500
H	-7.91615100	3.70014900	1.09133800
H	-7.92990000	2.13168700	-3.33171900
H	-7.87389700	2.43443000	3.21023500
H	-7.92510600	-0.19996700	-4.00255500
H	-7.86989200	0.21225900	4.16244800
H	-7.93195000	-2.45090200	-3.09644000
H	-7.87668400	-2.09519600	3.44291500
H	-7.93850500	-3.71554300	-1.00309600
H	-7.92053500	-3.56885800	1.46326400
H	7.86492100	-3.05671000	2.56344800
H	7.86766000	3.28459300	2.23843300
H	7.85982700	-1.03336000	3.96127000
H	7.86080100	1.41469500	3.83688800
H	7.88603500	3.91321500	-0.16514100
H	7.88208200	-3.92254300	0.23435600
H	7.89294500	3.06684000	-2.50066100
H	7.88909100	-3.31380900	-2.17370700
H	7.88810300	-1.42622400	-3.76077500
H	7.88976100	1.02684600	-3.88547500
N	-2.50427200	0.20987700	4.18170600
N	0.34515600	0.20718800	4.16202600
C	-0.23601300	0.05976300	-0.58371600
O	0.93346000	0.12649300	-0.53246800
O	-1.40552000	-0.00720400	-0.62389800

Table S25. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the exterior wall of [8,4]-SWNT.

C	-3.78066100	-3.89053600	-2.03821600
C	-5.14878400	-4.13527400	-1.62927000
C	3.83503800	-3.83863200	-2.05630400
C	1.11557100	-4.22170700	-1.17605000
C	-0.24537100	-4.33316800	-0.71298500
C	-1.33057100	-4.08568800	-1.62068500
C	-2.95232700	-4.38905300	0.23051900
C	-2.68409800	-4.24607100	-1.17120300
C	-4.32037100	-4.34761200	0.69733000
C	-5.40625500	-4.47983900	-0.22163500
C	-6.99635700	-4.18534700	1.63248600
C	-6.73674000	-4.56265300	0.32895000
C	5.98989800	-4.36347200	-0.26394100
C	6.24251300	-4.06659000	-1.62919500
C	4.63595400	-4.35304000	0.22089900
C	3.55730600	-4.29122700	-0.72346600
C	1.92614200	-4.21123000	1.15799100
C	2.19517400	-4.36277500	-0.25269700
C	0.56837200	-4.06528900	1.60706300

C	-0.51673000	-4.33092400	0.69768800
C	-2.14551600	-3.61434400	2.43747300
C	-1.87427300	-4.22914700	1.15926800
C	-3.50944800	-3.31639000	2.80227500
C	-4.58512900	-3.87771700	2.03599200
C	-6.19872100	-2.67043000	3.45881700
C	-5.94012700	-3.64186800	2.45610400
C	6.78898300	-4.01465700	2.02682700
C	7.04854300	-4.38102100	0.72008300
C	5.45681200	-3.66310500	2.45328100
C	4.37209300	-4.04582400	1.60608700
C	2.73058300	-2.98654800	3.14293300
C	3.00334900	-3.84648800	2.02792300
C	1.37452800	-2.62476700	3.44321000
C	0.29368400	-3.32382700	2.80609400
C	-1.34722900	-1.80230100	3.90571400
C	-1.06942700	-2.99657400	3.14368900
C	-2.70363400	-1.35865500	4.05825300
C	-3.79443900	-2.22966500	3.69471200
C	-5.43128200	-0.42021000	4.27484600
C	-5.16577000	-1.82658700	3.93121800
C	-6.76457700	0.12494900	4.34887700
C	6.22629000	-1.77985300	3.92972500
C	5.19305300	-2.62825800	3.46639200
C	3.53603900	-0.88529900	4.14072700
C	3.82180600	-2.21639200	3.68790600
C	2.17155000	-0.42016000	4.20531700
C	1.09641100	-1.34774100	4.05691300
C	-0.54444300	0.51908900	4.15847800
C	-0.26719300	-0.89046500	4.16101200
C	-1.90337900	0.97505400	4.04820600
C	-2.97863200	0.04186300	4.20068600
C	-4.61554400	1.84035100	3.67710400
C	-4.34829700	0.50314500	4.14988300
C	-5.97059800	2.25458500	3.43172700
C	-7.02705400	1.42714300	3.96900500
C	7.02098900	0.57249800	4.24917300
C	5.96643600	-0.41587900	4.22617200
C	4.34276300	1.44745200	3.90000200
C	4.61061100	0.06338200	4.20887200
C	2.97342800	1.86358700	3.69352200
C	1.89761800	0.98952800	4.05300300
C	0.26337600	2.62934100	3.15423700
C	0.53870400	1.43292900	3.89942800
C	-1.09908500	2.96035500	2.81762600
C	-2.17622200	2.25140300	3.43018100
C	-3.82068000	3.49973700	2.03159100
C	-3.53933900	2.61028100	3.12190800
C	-5.19033900	3.73100800	1.61992400
C	-6.22679000	3.25530000	2.45756400
C	6.75803700	1.87796100	3.88070800
C	5.16363900	3.30930600	2.48406000
C	5.42599700	2.29870100	3.52179300
C	3.79376000	3.52384400	2.06406900
C	2.70099200	2.97601300	2.83004900
C	1.07321400	3.87410900	1.17799000
C	-0.28809500	3.96788900	0.71261000

C	-2.99358100	4.00602700	-0.23571800
C	-2.72632900	3.86532000	1.16638000
C	-4.35989500	3.95101800	-0.70522200
C	-5.44861100	4.07280400	0.21187700
C	-7.03246500	3.76255300	-1.64493500
C	-6.77880000	4.14278700	-0.34107800
C	5.94616200	4.07061200	0.27506100
C	6.19940300	3.77624900	1.64076900
C	4.59328900	4.04603200	-0.21224800
C	3.51375400	3.97276500	0.73027800
C	1.88748200	3.87308600	-1.15392000
C	2.15223400	4.02735800	0.25653400
C	0.53266100	3.71277200	-1.60572000
C	-0.55707400	3.96441500	-0.69865700
C	-2.17527400	3.23982100	-2.44275300
C	-1.91298900	3.85438400	-1.16263800
C	-3.53558200	2.92846600	-2.80970700
C	-4.61772700	3.47872200	-2.04453700
C	-6.21700100	2.25527400	-3.46984300
C	-5.96965400	3.22929400	-2.46675000
C	6.75322500	3.73002500	-2.01412600
C	7.00648800	4.09893200	-0.70684400
C	5.42556900	3.36503700	-2.44311300
C	4.33531000	3.73630800	-1.59792700
C	2.70795600	2.66122100	-3.13933700
C	2.96965900	3.52277100	-2.02265200
C	1.35656500	2.28611900	-3.44328200
C	0.26740700	2.97343800	-2.80751100
C	-1.35639700	1.43617000	-3.90997100
C	-1.09187500	2.63300400	-3.14748900
C	-2.70800700	0.97878100	-4.06413700
C	-3.80817500	1.83892800	-3.70263700
C	-5.42556900	0.01294100	-4.28509000
C	-5.17491200	1.42193800	-3.94096400
C	-6.75310100	-0.54558600	-4.36204600
C	6.21709100	1.48957800	-3.91789200
C	5.17444700	2.32765700	-3.45699200
C	3.53642700	0.56800400	-4.13471500
C	3.80796600	1.90209600	-3.68184100
C	2.17679200	0.08910800	-4.20165300
C	1.09219100	1.00606700	-4.05672400
C	-0.52966600	-0.87721000	-4.15800600
C	-0.26662500	0.53502100	-4.16245700
C	-1.88412100	-1.34669300	-4.04978200
C	-2.96851300	-0.42454500	-4.20563600
C	-4.58830200	-2.23923500	-3.68535900
C	-4.33357700	-0.89944300	-4.15769000
C	-5.93971000	-2.66715900	-3.44308900
C	-7.00323100	-1.85040800	-3.98283600
C	7.03599700	-0.85464800	-4.23584900
C	5.97151700	0.12300900	-4.21481600
C	4.36597700	-1.75640400	-3.89090200
C	4.62052100	-0.36989000	-4.20005800
C	3.00045300	-2.18601400	-3.68587000
C	1.91663900	-1.32301800	-4.04772700
C	0.29744600	-2.97907200	-3.15095200
C	0.56203900	-1.77983400	-3.89572000

C	-1.06227100	-3.32415700	-2.81741300
C	-2.14516900	-2.62553400	-3.43187100
C	-3.50561200	-2.99813100	-3.12752200
C	-6.18810000	-3.67020800	-2.46932400
C	6.78546800	-2.16270300	-3.86794100
C	5.20333600	-3.60993100	-2.47393500
C	5.45711600	-2.59668300	-3.51116000
C	2.73764100	-3.30112400	-2.82295700
C	1.38485400	-3.60863800	-2.45525200
H	-7.25429500	1.99198600	-3.66734900
H	-7.22600600	-3.87233400	-2.21201400
H	-7.23889700	-2.41762400	3.65487900
H	-7.26607600	3.44729700	2.19812000
H	7.28091900	-3.94657600	-1.93185400
H	7.23847400	3.66681600	1.94519800
H	7.26654600	-2.07819200	3.81507900
H	7.25408400	1.79829100	-3.80107600
H	-7.58901200	0.09546600	-4.63713000
H	-8.02610400	-2.22542200	-3.95671400
H	-7.56768400	-4.84088800	-0.31716200
H	-8.02159400	-4.16379400	2.00128700
H	-7.59458500	-0.52449200	4.62209200
H	-8.05358200	1.79185800	3.94058300
H	-7.61347000	4.41344800	0.30341400
H	-8.05679300	3.73106200	-2.01555400
H	7.58761200	2.57483700	3.77403500
H	7.62175800	-2.85127800	-3.75981100
H	8.05925300	-0.52174200	-4.40819300
H	8.04722100	0.24989900	4.42341300
H	8.07437200	-4.54970400	0.39326400
H	7.62084400	-3.90415500	2.72036900
H	8.02988800	4.27812800	-0.37802600
H	7.58744000	3.62794000	-2.70613900
C	1.34576200	3.26921400	2.46007300
C	-1.37297600	3.71516800	1.61831800
C	-0.27231700	7.12616600	-0.00349500
O	0.79202300	7.11341700	-0.49466800
O	-1.33658700	7.15020800	0.48743900

Table S26. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the interior wall of [8,4]-SWNT.

C	-4.21663700	0.01257700	-3.80788800
C	-4.22590900	0.48683600	-5.17695500
C	-4.21499300	-0.01326000	3.80815700
C	-4.11010000	0.93673200	1.08677800
C	-3.97504000	1.39214700	-0.27442500
C	-4.19525800	0.47706100	-1.35888700
C	-3.55189500	2.23828900	-2.98060500
C	-4.11070800	0.94508800	-2.71268600
C	-3.28274700	2.62420100	-4.34751800
C	-3.84080500	1.88406600	-5.43517500
C	-2.67560700	3.36111800	-7.02084000
C	-3.63965800	2.40480000	-6.76508000
C	-3.81744800	1.81406000	5.96121900
C	-4.21977200	0.47612100	6.21480600
C	-3.56629700	2.22983500	4.60752900

C	-3.96390300	1.37155400	3.52874000
C	-2.97297300	2.97344800	1.89897300
C	-3.79153800	1.81494500	2.16652300
C	-2.61945400	3.29083700	0.54220400
C	-3.28637100	2.62263900	-0.54495300
C	-1.80795600	3.79171400	-2.16718800
C	-2.96624700	2.97372800	-1.90104200
C	-1.36457400	3.96476200	-3.52867400
C	-2.22137700	3.56631300	-4.60804400
C	-0.46860200	4.22398600	-6.21331700
C	-1.80533500	3.81830400	-5.96133300
C	-2.40732500	3.65115700	6.76289500
C	-3.36253700	2.68644200	7.01992800
C	-1.88530400	3.84965000	5.43344800
C	-2.62515600	3.29168300	4.34598900
C	-0.94422900	4.11624500	2.71129800
C	-2.23858400	3.56010100	2.97898600
C	-0.47499600	4.19901700	1.35757100
C	-1.38818800	3.97789800	0.27219200
C	0.48239300	4.20072500	-1.35800600
C	-0.93150800	4.11217500	-1.08774200
C	0.95046500	4.11661800	-2.71094400
C	0.01888100	4.21948300	-3.80663000
C	1.89084300	3.85052100	-5.43268700
C	0.49291200	4.23076500	-5.17524300
C	2.41381500	3.65299800	-6.76192500
C	0.47391200	4.22610100	6.21443100
C	-0.48782100	4.23141500	5.17610200
C	1.37150300	3.96895700	3.52951500
C	-0.01296300	4.22168000	3.80747000
C	1.81613400	3.79733700	2.16763300
C	0.93987100	4.11594400	1.08662200
C	2.62772800	3.29687400	-0.54343300
C	1.39703000	3.98412400	-0.27374500
C	2.97881200	2.97635600	-1.89895400
C	2.24408800	3.56150500	-2.97840800
C	3.57057300	2.23064100	-4.60634200
C	2.62990300	3.29251400	-4.34513000
C	3.82270900	1.81526100	-5.95976100
C	3.36903400	2.68832500	-7.01850300
C	2.68019600	3.36085300	7.02207500
C	1.81081700	3.81968700	5.96249600
C	3.28889700	2.62635700	4.34808000
C	2.22777700	3.56888300	4.60908900
C	3.55792800	2.24083600	2.98062500
C	2.97382300	2.97799800	1.90074400
C	3.97410900	1.39242800	0.27353800
C	3.29198000	2.62644200	0.54369400
C	4.10765900	0.93730200	-1.08701500
C	3.79251400	1.81580700	-2.16580200
C	4.21575000	-0.01230300	-3.80686800
C	3.96526100	1.37194400	-3.52739300
C	4.22629600	-0.48569300	-5.17605000
C	4.22344100	0.47722300	-6.21304100
C	3.64342300	2.40361200	6.76566300
C	4.22952400	0.48698400	5.17644100
C	3.84520300	1.88406300	5.43539600

C	4.21861600	0.01286600	3.80712100
C	4.11261500	0.94573700	2.71196900
C	4.10949400	-0.93758800	1.08655600
C	3.97432800	-1.39262000	-0.27437500
C	3.55561300	-2.23949500	-2.98121900
C	4.10965700	-0.94486900	-2.71228700
C	3.28737400	-2.62533900	-4.34848500
C	3.84339900	-1.88307300	-5.43531300
C	2.68100000	-3.36109800	-7.02221200
C	3.64392300	-2.40387300	-6.76531100
C	3.82316400	-1.81362500	5.96176800
C	4.22837700	-0.47615500	6.21403600
C	3.57145700	-2.23024200	4.60828200
C	3.96829400	-1.37241400	3.52844700
C	2.98113800	-2.97835800	1.89969200
C	3.79572200	-1.81690400	2.16644800
C	2.62922500	-3.29874200	0.54323800
C	3.29258200	-2.62717900	-0.54456000
C	1.81563100	-3.79759100	-2.16858400
C	2.97305700	-2.97782500	-1.90175800
C	1.37097800	-3.96954100	-3.53038800
C	2.22731400	-3.56909000	-4.60967400
C	0.47395500	-4.22612400	-6.21524700
C	1.81091100	-3.82017700	-5.96317000
C	2.41051500	-3.64854500	6.76520100
C	3.36686900	-2.68446800	7.02139800
C	1.89004500	-3.84994000	5.43528600
C	2.63121000	-3.29347800	4.34733400
C	0.95092400	-4.11934500	2.71225200
C	2.24588600	-3.56394200	2.98012500
C	0.48235500	-4.20336000	1.35839800
C	1.39741900	-3.98595000	0.27331800
C	-0.47572500	-4.20074600	-1.35864100
C	0.93968000	-4.11740600	-1.08762700
C	-0.94513200	-4.11746800	-2.71241600
C	-0.01344400	-4.22250000	-3.80839900
C	-1.88571600	-3.84972600	-5.43474100
C	-0.48796100	-4.23238000	-5.17714800
C	-2.40689000	-3.64972300	-6.76457900
C	-0.46993400	-4.22779400	6.21480000
C	0.49257000	-4.23269100	5.17696800
C	-1.36599900	-3.96792400	3.52953200
C	0.01831400	-4.22221100	3.80788000
C	-1.80974500	-3.79505800	2.16768400
C	-0.93278400	-4.11556900	1.08750300
C	-2.62152400	-3.29314100	-0.54318000
C	-1.38984300	-3.98077100	-0.27319800
C	-2.97446000	-2.97482200	-1.89997400
C	-2.23955800	-3.56118300	-2.97992300
C	-3.56745700	-2.23009100	-4.60820500
C	-2.62596700	-3.29225100	-4.34707000
C	-3.81864900	-1.81368100	-5.96189800
C	-3.36247700	-2.68518100	-7.02115700
C	-2.67596500	-3.36166000	7.02196800
C	-1.80639200	-3.82002000	5.96246200
C	-3.28362800	-2.62563400	4.34820800
C	-2.22253800	-3.56807200	4.60899000

C	-3.55408600	-2.24055300	2.98109500
C	-2.96809100	-2.97601500	1.90108200
C	-3.97658600	-1.39369300	0.27408000
C	-3.28859100	-2.62483300	0.54443200
C	-4.11146700	-0.93809400	-1.08714100
C	-3.79324300	-1.81629700	-2.16695000
C	-3.96576200	-1.37238400	-3.52912100
C	-4.22261700	-0.47598300	-6.21456100
C	-3.63894800	-2.40433300	6.76578700
C	-4.22314500	-0.48693000	5.17741500
C	-3.83950800	-1.88390500	5.43593500
C	-4.11069600	-0.94612100	2.71297000
C	-4.19527500	-0.47834000	1.35888800
H	0.15194400	-4.27269400	-7.25377000
H	-4.26914400	-0.15446400	-7.25338300
H	-0.14689500	4.27172800	-7.25172500
H	4.27102400	0.15654100	-7.25181400
H	-4.26728800	0.15532500	7.25365800
H	4.27663400	-0.15503500	7.25289400
H	0.15216500	4.27362600	7.25287100
H	-0.14857400	-4.27582900	7.25347400
H	-1.97868500	-4.20485100	-7.59751500
H	-3.67458000	-2.48412500	-8.04584300
H	-4.19360500	1.97573300	-7.59848100
H	-2.47398700	3.67281000	-8.04538500
H	1.98659200	4.20919000	-7.59447300
H	3.68184400	2.48799100	-8.04293400
H	4.19785700	-1.97418400	-7.59816800
H	2.47983700	-3.67250400	-8.04701100
H	4.19483000	1.97179500	7.59936700
H	-4.19093100	-1.97324200	7.59937800
H	-2.47332500	-3.67152500	8.04692300
H	2.47693300	3.66996900	8.04712600
H	-3.67289200	2.48464600	8.04486600
H	-1.97829400	4.20540600	7.59590000
H	3.67723700	-2.48201600	8.04633200
H	1.98040800	-4.20141100	7.59876200
C	4.19279200	0.47707700	1.35801100
C	4.19113100	-0.47683600	-1.35856800
C	0.47708400	0.00120700	0.01233000
O	0.47300300	-0.69271000	0.95706000
O	0.47643000	0.69459800	-0.93187700

Table S27. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the exterior wall of [8,4]-N-SWNT.

C	-4.25640200	0.00906700	-3.81575600
C	-4.27486200	0.48676100	-5.18274200
C	-4.22630500	-0.01850700	3.81379400
C	-4.12779100	0.92915400	1.08613100
C	-4.00441700	1.38825600	-0.27297000
C	-4.22057500	0.46956500	-1.35916200
C	-3.60272900	2.23466200	-2.98903800
C	-4.14588100	0.94071600	-2.71888700
C	-3.34378600	2.62309300	-4.35555100
C	-3.90537900	1.87736600	-5.44047600
C	-2.74796300	3.35023500	-7.03869100

C	-3.71270300	2.40240000	-6.77560100
C	-3.80214500	1.79388400	5.97442400
C	-4.22151100	0.47022800	6.22613400
C	-3.55777100	2.21570400	4.61660500
C	-3.96833500	1.36686500	3.53761400
C	-2.98408900	2.95743600	1.90124500
C	-3.79753300	1.81166900	2.17238400
C	-2.64807700	3.28737400	0.53906600
C	-3.32000300	2.62213300	-0.54520700
C	-1.85873000	3.78796900	-2.18325900
C	-3.00525100	2.97376700	-1.90703900
C	-1.41821800	3.95700300	-3.54986000
C	-2.27718400	3.55734400	-4.62408200
C	-0.52611000	4.18939900	-6.24448000
C	-1.85750100	3.79618100	-5.98362700
C	-2.36068900	3.60771900	6.77684100
C	-3.32914900	2.66337500	7.03588400
C	-1.84476400	3.80790200	5.43873600
C	-2.60854100	3.26996600	4.35367100
C	-0.94356600	4.08329100	2.71144300
C	-2.23264900	3.54173400	2.98567400
C	-0.49175600	4.18327600	1.34400000
C	-1.42032500	3.97981100	0.26140600
C	0.43489000	4.19111500	-1.38030500
C	-0.97219200	4.11498500	-1.10014400
C	0.90191400	4.09594500	-2.74097000
C	-0.03092700	4.19990800	-3.83593500
C	1.83536400	3.81135600	-5.45774000
C	0.44493600	4.19005500	-5.20382800
C	2.36829300	3.60551200	-6.79410800
C	0.52866700	4.16771200	6.20440500
C	-0.45602300	4.17616600	5.17305700
C	1.38504800	3.93290500	3.50888800
C	0.00220100	4.18249300	3.80063200
C	1.80505500	3.75976300	2.13612100
C	0.90628900	4.09689100	1.05901200
C	2.57234500	3.26511200	-0.57624900
C	1.35310900	3.97528700	-0.29806600
C	2.91986600	2.94707500	-1.92294500
C	2.19058100	3.54303600	-3.01066500
C	3.54814600	2.22173200	-4.61944500
C	2.58455000	3.27535800	-4.37040600
C	3.81449700	1.79798700	-5.97549400
C	3.34432500	2.66970500	-7.04308500
C	2.77131900	3.35274100	6.98067300
C	1.85703300	3.77991500	5.93391800
C	3.35098200	2.62779200	4.29162800
C	2.26429400	3.54347900	4.56761600
C	3.58613700	2.23206900	2.92113500
C	2.92930000	2.94591400	1.85496500
C	3.93416100	1.37144400	0.23149100
C	3.23221600	2.58270400	0.49850300
C	4.05629600	0.92370700	-1.10564900
C	3.72466900	1.79274300	-2.18060900
C	4.26124300	0.00053200	-3.80592500
C	3.94728000	1.37699600	-3.54706700
C	4.27801000	-0.48694200	-5.16936500

C	4.26298100	0.48840000	-6.21712200
C	3.75091600	2.42608300	6.70913200
C	4.31553200	0.52223700	5.10090600
C	3.94447000	1.90458700	5.36911100
C	4.29062900	0.03514100	3.73799100
C	4.14713700	0.96112400	2.64361100
C	4.06535500	-0.88863900	1.03799100
C	3.93451400	-1.33510700	-0.29908200
C	3.57314200	-2.20057400	-2.98373600
C	4.12878500	-0.92541000	-2.70932700
C	3.32980900	-2.59718000	-4.35235000
C	3.91219800	-1.87158700	-5.43437100
C	2.73345700	-3.32565900	-7.03680000
C	3.71045200	-2.39392400	-6.77259100
C	3.86976900	-1.76498200	5.91012500
C	4.31260300	-0.45343200	6.14876700
C	3.59469400	-2.18932900	4.55573500
C	3.98124700	-1.34263900	3.48102600
C	2.94735900	-2.91723000	1.86470300
C	3.74665600	-1.75796600	2.11622700
C	2.59118800	-3.23738100	0.52050400
C	3.23917400	-2.55264000	-0.55962200
C	1.80620600	-3.73864100	-2.18559400
C	2.92796400	-2.91724800	-1.91334700
C	1.37661700	-3.91313300	-3.55486300
C	2.24575800	-3.51856200	-4.62018600
C	0.50088200	-4.15260400	-6.24356700
C	1.82924700	-3.75724600	-5.98328700
C	2.43983900	-3.58034000	6.74004500
C	3.41268900	-2.63949600	6.98130300
C	1.89705500	-3.78812900	5.40760800
C	2.63457900	-3.24824000	4.31449000
C	0.94342100	-4.07845300	2.69844500
C	2.23078000	-3.51778100	2.95804600
C	0.46615100	-4.17613500	1.34148400
C	1.37464500	-3.95567100	0.25198400
C	-0.48201600	-4.17423900	-1.37562300
C	0.91800400	-4.07990600	-1.10170100
C	-0.94486400	-4.07642300	-2.73938400
C	-0.00713600	-4.17027600	-3.83592500
C	-1.86875800	-3.80559800	-5.45949500
C	-0.47586900	-4.16619200	-5.20484800
C	-2.39615400	-3.60785000	-6.79339200
C	-0.45578200	-4.17872200	6.21319800
C	0.50682900	-4.17463900	5.16476000
C	-1.37076100	-3.95195100	3.52565000
C	0.02004000	-4.18735900	3.80072200
C	-1.82296600	-3.78531800	2.16250800
C	-0.94342600	-4.10804400	1.07242700
C	-2.63630100	-3.28904700	-0.55367900
C	-1.40286200	-3.97518700	-0.28571300
C	-2.98462900	-2.96085100	-1.91321800
C	-2.23906400	-3.54148300	-3.00345100
C	-3.58322900	-2.22192600	-4.62388700
C	-2.62678300	-3.27149000	-4.36845400
C	-3.84034500	-1.80123700	-5.97970400
C	-3.37146500	-2.66843200	-7.04481200

C	-2.67561400	-3.35147300	7.02496200
C	-1.79132000	-3.79285400	5.96285300
C	-3.29663800	-2.62789000	4.34645300
C	-2.22308100	-3.55653000	4.60663700
C	-3.56832600	-2.24086600	2.98197200
C	-2.97577600	-2.97709200	1.89527100
C	-3.99554000	-1.39663300	0.26908600
C	-3.30289100	-2.62705900	0.53591600
C	-4.13182700	-0.93815700	-1.08905900
C	-3.80601500	-1.81904600	-2.17789200
C	-3.98953100	-1.37506500	-3.54165900
C	-4.26828800	-0.47963500	-6.22803300
C	-3.64740200	-2.40881300	6.76943500
C	-4.23177000	-0.49619000	5.18087100
C	-3.85317600	-1.88485500	5.43578000
C	-4.11987000	-0.94965500	2.71608000
C	-4.20754500	-0.47894800	1.35694000
H	0.18238700	-4.19759100	-7.28311300
H	-4.32953900	-0.15482100	-7.26476400
H	-0.20612800	4.23493800	-7.28365300
H	4.32960800	0.15774600	-7.25132700
H	-4.27318800	0.14520000	7.26331900
H	4.38651400	-0.12277300	7.18247500
H	0.21783100	4.21113300	7.24633500
H	-0.12735400	-4.22247600	7.24980100
H	-1.96152200	-4.15869700	-7.62593500
H	-3.69658200	-2.47459200	-8.06670500
H	-4.28427400	1.98328300	-7.60212000
H	-2.55652200	3.66847100	-8.06319100
H	1.94322800	4.16287300	-7.62736600
H	3.67838300	2.48192500	-8.06306200
H	4.29795100	-1.99118100	-7.59629400
H	2.54470700	-3.64897200	-8.06007900
H	4.34699500	2.02636800	7.52810500
H	-4.21472300	-1.99267700	7.60036600
H	-2.47439400	-3.66863200	8.04791700
H	2.58874200	3.67528600	8.00531700
H	-3.64537000	2.46799100	8.06027200
H	-1.92240900	4.16098000	7.60585800
H	3.75459300	-2.45058000	7.99846300
H	2.02498200	-4.14088200	7.57627500
N	4.23376100	-0.46493700	-1.38167600
N	4.25416300	0.50249800	1.31267000
C	7.26332300	-0.28773400	1.06835500
O	7.30629100	-0.62971200	2.18846500
O	7.22476200	0.05295700	-0.05309700

Table S28. B971/6-31G(d)-DCP optimized coordinates (Å) for CO_2 bound to the interior wall of [8,4]-N-SWNT.

C	-4.23955500	0.01306300	-3.81494500
C	-4.25116400	0.49077400	-5.18193300
C	-4.23955200	-0.01362800	3.81513600
C	-4.12732100	0.93326200	1.08766600
C	-3.99677200	1.39131300	-0.27113600
C	-4.21144700	0.47358900	-1.35824600
C	-3.58149700	2.23597100	-2.98564300

C	-4.13012400	0.94428100	-2.71770200
C	-3.31639300	2.62383400	-4.35099600
C	-3.87612400	1.88009300	-5.43817700
C	-2.70794300	3.34960500	-7.03157100
C	-3.67659600	2.40467200	-6.77252400
C	-3.81981800	1.79782000	5.97724900
C	-4.24321100	0.47519000	6.22737400
C	-3.56901700	2.21898700	4.62037600
C	-3.97738400	1.37105200	3.53988700
C	-2.98120700	2.95758200	1.90714000
C	-3.79955300	1.81494600	2.17529700
C	-2.63789400	3.28519200	0.54613400
C	-3.30677400	2.62207000	-0.54090300
C	-1.83588500	3.78286400	-2.17266500
C	-2.98538900	2.97240400	-1.90124800
C	-1.39025000	3.95146300	-3.53741300
C	-2.24604000	3.55487000	-4.61506900
C	-0.48715500	4.18292800	-6.22827800
C	-1.82051200	3.79296700	-5.97288000
C	-2.37661100	3.60780500	6.78517400
C	-3.34884000	2.66633200	7.04045200
C	-1.85460200	3.80623700	5.44917200
C	-2.61564700	3.27037200	4.36113800
C	-0.94121700	4.07716200	2.72550500
C	-2.23317300	3.54026900	2.99464500
C	-0.48351300	4.17472500	1.35981700
C	-1.40730400	3.97343000	0.27313400
C	0.45425100	4.18115700	-1.36044000
C	-0.95338800	4.10781300	-1.08620400
C	0.92597900	4.08445500	-2.71893900
C	-0.00165400	4.19119700	-3.81771500
C	1.87000600	3.79952400	-5.43191200
C	0.47952900	4.18117500	-5.18361700
C	2.40835000	3.59368500	-6.76619600
C	0.51722600	4.15829400	6.22424400
C	-0.46354400	4.16958700	5.18917800
C	1.38312600	3.92006300	3.53230500
C	0.00008700	4.17414500	3.81858700
C	1.80764200	3.74556900	2.16136300
C	0.91498500	4.08469900	1.08020700
C	2.58481700	3.25023400	-0.54818600
C	1.36720700	3.96387100	-0.27501900
C	2.93658400	2.93119000	-1.89303200
C	2.21372500	3.52866300	-2.98349400
C	3.57521300	2.20583800	-4.58725900
C	2.61299900	3.26129800	-4.34167000
C	3.84651200	1.78231800	-5.94250600
C	3.38319900	2.65581000	-7.01165600
C	2.75492700	3.33728400	7.00906900
C	1.84546700	3.76625300	5.95894700
C	3.34309500	2.61040400	4.32227200
C	2.25738400	3.52840200	4.59426100
C	3.58258200	2.21440600	2.95275200
C	2.93008500	2.92808400	1.88466200
C	3.93628000	1.35183700	0.26525400
C	3.23669600	2.56508200	0.52904200
C	4.06417800	0.90574600	-1.07210700

C	3.73867100	1.77521300	-2.14788700
C	4.28041000	-0.01680000	-3.77188900
C	3.96754200	1.36003700	-3.51363900
C	4.30076900	-0.50398500	-5.13541400
C	4.29231800	0.47174200	-6.18297300
C	3.73372300	2.40858400	6.74119700
C	4.30082200	0.50345900	5.13557500
C	3.93183400	1.88677300	5.40213200
C	4.28044200	0.01627800	3.77205500
C	4.14249400	0.94218200	2.67637700
C	4.06406500	-0.90623900	1.07226300
C	3.93618000	-1.35230500	-0.26511600
C	3.58253100	-2.21493500	-2.95258900
C	4.14245200	-0.94270300	-2.67621300
C	3.34303500	-2.61093300	-4.32210500
C	3.93176200	-1.88729500	-5.40196900
C	2.75485700	-3.33781400	-7.00890200
C	3.73364400	-2.40910400	-6.74103400
C	3.84652600	-1.78283400	5.94267100
C	4.29235500	-0.47226700	6.18313600
C	3.57520400	-2.20634300	4.58742600
C	3.96752500	-1.36054100	3.51380900
C	2.93653000	-2.93166700	1.89321800
C	3.73862200	-1.77570800	2.14806200
C	2.58472200	-3.25064300	0.54836100
C	3.23660400	-2.56555100	-0.52890600
C	1.80760700	-3.74614300	-2.16119700
C	2.93003600	-2.92862300	-1.88451100
C	1.38308100	-3.92064100	-3.53213300
C	2.25733000	-3.52894900	-4.59409000
C	0.51717200	-4.15886000	-6.22406600
C	1.84541000	-3.76679900	-5.95877500
C	2.40835200	-3.59418700	6.76636800
C	3.38321200	-2.65632400	7.01182300
C	1.86999500	-3.80001500	5.43208800
C	2.61297900	-3.26179200	4.34184400
C	0.92595200	-4.08492900	2.71912700
C	2.21369900	-3.52915700	2.98367200
C	0.45419600	-4.18160300	1.36064000
C	1.36710900	-3.96425300	0.27519500
C	-0.48357200	-4.17531300	-1.35964000
C	0.91493000	-4.08521600	-1.08004600
C	-0.94127900	-4.07777400	-2.72532600
C	0.00003600	-4.17473400	-3.81840500
C	-1.85465800	-3.80682500	-5.44898900
C	-0.46359600	-4.17017000	-5.18899700
C	-2.37666000	-3.60838200	-6.78499200
C	-0.48715800	-4.18343600	6.22846500
C	0.47951800	-4.18166800	5.18380000
C	-1.39026800	-3.95197900	3.53760700
C	-0.00167100	-4.19168300	3.81790100
C	-1.83592400	-3.78340500	2.17286700
C	-0.95343900	-4.10834600	1.08640300
C	-2.63796800	-3.28579700	-0.54594700
C	-1.40736000	-3.97400800	-0.27294900
C	-2.98128600	-2.95819600	-1.90695700
C	-2.23324500	-3.54088300	-2.99446000

C	-3.56906300	-2.21956600	-4.62019000
C	-2.61570900	-3.27096800	-4.36095300
C	-3.81984800	-1.79838400	-5.97706400
C	-3.34887900	-2.66689800	-7.04027000
C	-2.70795500	-3.35014800	7.03176700
C	-1.82052100	-3.79349700	5.97307500
C	-3.31642200	-2.62439100	4.35119300
C	-2.24605700	-3.55540700	4.61526700
C	-3.58153000	-2.23653700	2.98584000
C	-2.98544000	-2.97297800	1.90144500
C	-3.99681400	-1.39189600	0.27132400
C	-3.30683400	-2.62266200	0.54109600
C	-4.12736300	-0.93384600	-1.08747900
C	-3.79961800	-1.81554100	-2.17511100
C	-3.97742500	-1.37162900	-3.53969900
C	-4.24321600	-0.47574500	-6.22718700
C	-3.67662000	-2.40522600	6.77272000
C	-4.25117800	-0.49133100	5.18212500
C	-3.87615100	-1.88065200	5.43837300
C	-4.13013700	-0.94484800	2.71789400
C	-4.21144800	-0.47416500	1.35843600
H	0.20249400	-4.20341400	-7.26478900
H	-4.29958200	-0.15083600	-7.26416400
H	-0.16287600	4.22814900	-7.26613800
H	4.36215200	0.14123400	-7.21702200
H	-4.29958400	0.15028500	7.26435100
H	4.36220400	-0.14175900	7.21718200
H	0.20255200	4.20284900	7.26496800
H	-0.16287100	-4.22865500	7.26632200
H	-1.94014700	-4.16051400	-7.61569400
H	-3.66978700	-2.47259200	-8.06340200
H	-4.24617700	1.98742500	-7.60135500
H	-2.51149600	3.66744500	-8.05525000
H	1.98827900	4.15280600	-7.60080200
H	3.72128000	2.46789600	-8.03028000
H	4.32554200	-2.00816900	-7.56246300
H	2.56908100	-3.66069100	-8.03285800
H	4.32563000	2.00765600	7.56262200
H	-4.24620400	-1.98798400	7.60155100
H	-2.51150400	-3.66798500	8.05544600
H	2.56915600	3.66016200	8.03302500
H	-3.66975700	2.47203900	8.06358300
H	-1.94010000	4.15994200	7.61587300
H	3.72131000	-2.46842100	8.03044300
H	1.98828600	-4.15331000	7.60097300
N	4.24916400	-0.48325200	-1.34713900
N	4.24920000	0.48274600	1.34729700
C	0.38919000	0.00360400	0.01390700
O	0.38934300	-0.67551000	0.96963600
O	0.39597700	0.68260300	-0.94189100

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