Supporting Information

Supporting Information for the paper entitled "Carbon nanotubes adsorb U atoms differently in their inner and outer surfaces" by Minsi Xin, Xing Dai, Jie Han, Mingxing Jin, Camilo A. Jimenez-Cruz, Dajun Ding, Zhigang Wang, and Ruhong Zhou.

1. Electronic state as well as the corresponding energy and relative energy of U-CNT(inner) and U-CNT(outer) system

In this work, we considered three different adsorption sites of the U atoms: on top of C atoms, on top of the hole site of hexatomic ring, and on top of the C-C bond bridge. We first optimized the three types of conformations using 3-21G basis set in order to select the lowest energy structures of internal and external adsorption (see Table S1). We then reoptimized these lowest energy structures with a larger basis set 6-31G*, (see Table S2), and analyzed their electronic structures.

Table S1a Energies of the three adsorption sites of internal adsorption systems [a].

Multiplicity	BP86/3-21G			PBE/3-21G		
	Bridge	Hole	Top	Bridge	Hole	Top
3	-4657.95185	-4657.94914	—	-4652.77508	-4652.77197	—
5	**-4657.95386**	-4657.94621	—	**-4652.77724**	-4652.76903	—
7	-4657.94603	-4657.93531	—	-4652.76853	-4652.75804	—

[a] The adsorption structure of U atoms on top site of CNT internal surface is unstable.

Table S1b Energies of the three adsorption sites of external adsorption systems [b].

Multiplicity	BP86/3-21G			PBE/3-21G		
	Bridge	Hole	Top	Bridge	Hole	Top
3	-4657.81221	-4657.85064	-4657.82513	-4652.62535	-4652.66519	-4652.64183
5	-4657.82166	**-4657.85596**	-4657.82870	-4652.63808	**-4652.67448**	-4652.64360
7	-4657.82052	-4657.84246	—	-4652.64057	-4652.65699	—

[b] The septet of U atoms adsorbed on top site of CNT external surface structure is unstable.

In the actual calculations, we did not observe the structure of the U atom adsorbed on the top site of CNT internal surface, nor the structure with septet spin on the top site of CNT external surface. Other structures were obtained, with their energy presented in Table S1.

Table S2 Relative energy of the stable adsorption sites of both adsorption systems. (Set the total energy of the ground state as zero)

State	U-CNT (inner)			
	Energy (eV)			
	BP86/3-21G	BP86/6-31G(d)	PBE/3-21G	PBE/6-31G(d)
$^3A_1(^3A')$	0.05	0.06	0.06	0.07
$^3A''$	0.15	0.12	0.16	0.13
$^3A_2$	0.16	0.13	0.16	0.14
$^3B_1$	0.29	0.29	0.30	0.29
$^3B_2$	0.22	0.20	0.23	0.21
$^5A_1(^5A')$	**0**	**0**	**0**	**0**
$^5A''$	0.03	0.03	0.03	0.03
$^5A_2$	0.03	0.03	0.03	0.03
$^5B_1$	0.43	0.38	0.46	0.42
$^5B_2$	0.37	0.31	0.40	0.35
$^7A_1(^7A')$	0.21	0.15	0.24	0.18
$^7A''$	0.32	0.28	0.33	0.30
$^7A_2$	0.38	0.35	0.38	0.36
$^7B_1$	0.66	0.59	0.69	0.63
$^7B_2$	0.38	0.32	0.40	0.34

U-CNT (outer)				
State	Energy (eV)			
	BP86/3-21G	BP86/6-31G(d)	PBE/3-21G	PBE/6-31G(d)
$^3A_1$	2.82	1.10	3.06	1.28
$^3A_2$	2.86	1.14	3.10	1.33
$^3B_1$	2.93	1.16	3.17	1.37
$^3B_2$	2.81	1.09	3.05	1.27
$^5A_1$	2.73	1.00	2.98	1.18
$^5A_2$	2.59	0.86	2.83	1.04
$^5B_1$	2.66	0.93	2.90	1.11
$^5B_2$	**2.56**	**0.84**	**2.80**	**1.01**
$^7A_1$	3.07	1.29	3.32	1.47
$^7A_2$	3.78	2.04	4.01	2.21
$^7B_1$	3.21	1.69	3.46	1.87
$^7B_2$	3.03	1.26	3.27	1.45

Here 3-21G and 6-31G(d) given in Table S1 represent the basis set used on C atoms. The respective structures were optimized based on these different basis functions.

From Table S2 we can see that, the four methods all predict the same ground state. For the same basis set, the functional has small influence on the energy difference between electronic states, which is on the magnitude of 0.1 eV. For the same functional, the size of basis set presents a more apparent effect, however, the overall trend is the same. All of above illustrate the method we choose is reliable.

2. Calculation for the U adsorption system on the (5, 5) type single-walled carbon nanotube containing 8 six-membered ring with 3-21G

As an initial model, the (5, 5) type single-walled carbon nanotube containing 8 six-membered rings with H saturation at the ends (19.8 Å) adsorbs a U atom in the middle position of CNT's inner and exterior surfaces, respectively. Considering the extensive computational resources needed, we used BP86/3-21G method to perform the calculations. In order to compare the effects of CNT length on the electronic structures, as well as on charge transfer and interaction energy, we also reoptimized the geometries of adsorption systems (12.4 Å) in the main text based on BP86/3-21G method. Similar results were obtained by the analysis of the electronic structure and bonding nature of both adsorption systems.

(1) Structure

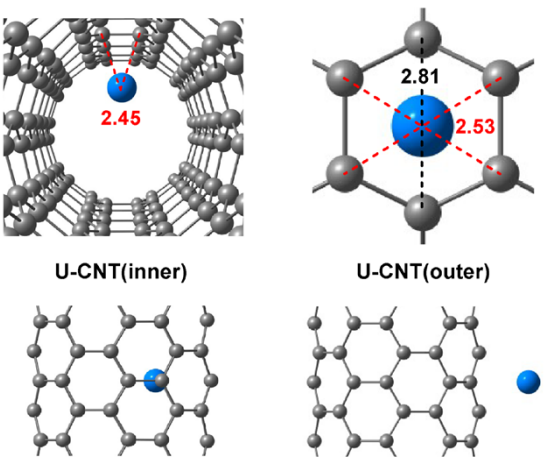

Fig. S1 Optimized structures of U atoms adsorbed on the 19.8 Å long CNT (inner, left) and U-CNT (outer, right).

Table S3 Relative energy of the stable adsorption sites of both adsorption systems. (Set the ground state energy of each individual system as zero)

System		Stable adsorption sites	El. state	Relative energy (eV)
U-CNT (12.4 Å)	inner	Bridge	$^3A_1$	0.05
			$^5A_1$	0
			$^7A_1$	0.21
	outer	Hole	$^3B_2$	2.81
			$^5B_2$	2.56
			$^7B_2$	3.03
U-CNT (19.8 Å)	inner	Bridge	$^3A_1$	0.05
			$^5A_1$	0
			$^7A_1$	0.20
	outer	Hole	^3A	2.86
			^5A	2.62
			^7A	3.02

After optimization of U atoms adsorbed on the 19.8 Å long CNT, we obtained the stable system structure as shown in Fig. S1. For internal adsorption, the U atom adsorbed on the bridge site is the most stable, and its quintet energy is minimum (U-CNT(inner)). The distance between the U atom and its adsorbed two C atoms on the C-C bond is 2.45 Å. While for the case of external adsorption, the U atom adsorbed on the hole is the most stable, and the ground state is quintet (U-CNT(outer)). The distance between the U atom and six C atoms on the six-membered ring adsorbed are 2.81 and 2.53 Å, respectively. From Table S3 we can see that, the stable sites of U atoms adsorbed on internal and external surfaces of 19.8 Å long CNT are similar to the stable sites of 12.4 Å long CNT, respectively, and all of ground electronic states are quintet.

(2) Spin density

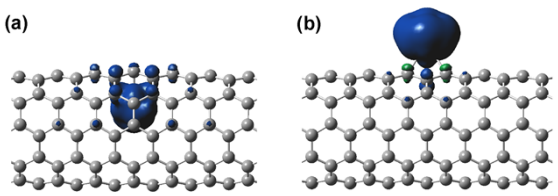

Fig. S2 Spin density distribution in the ground state of U atoms adsorbed on the 19.8 Å long CNT (inner, a) and (outer, b) systems. The blue area represents the net spin-up electrons, and the green area indicates the net spin-down electrons. Isovalue = 0.002.

Fig. S2(a) shows that, for the system of U atoms adsorbed on the internal surface of 19.8 Å long CNT, the quintet spin state can be attributed to the ferromagnetic coupling (blue region) between the net spin electrons of the inner U atom and external CNT, while the U atom contributes the majority. Further analysis on the spin density indicates that the number of net spin electrons on the U atom is +3.13 e, while that on CNT is +0.87 e. That is, from the six spin-up electrons on the U atom, three are donated to the CNT, among which two spin up, and one spins down. After ferromagnetic coupling of two parts of the unpaired-electrons, the total net spin electrons number of the system is +4 e, resulting in the quintet ground electronic state. For the U-CNT (outer) system, as shown in Fig. S2(b), the formation of ground state quintet is mostly from the contribution of the U atom. Spin density analysis indicates that there are +3.98 e single electrons on the U atom, but the CNT has nearly no net spin electrons (+0.02 e). It can be speculated that the U atom donates two electrons to the CNT, which are arranged in reverse, and the net spin on the CNT is almost zero.

(3) Electron density distribution and interaction energy

Table S4 The net charge on U atoms of the two U-CNT systems using Mulliken charge analysis and NPA.

Charge (e)	U-CNT(12.4 Å)		U-CNT(19.8 Å)	
	inner	outer	inner	outer
Mulliken	+2.44	+1.39	+2.42	+1.45
NPA	+1.18	+1.13	+1.16	+1.18

We calculated the net charge on U atoms of these adsorption structures U-CNT with a length of 12.4 Å and 19.8 Å, respectively, as shown in Table S4. With increase of the CNT length, the net charge on the U atom reduced slightly in the internal adsorption structures, and increased slightly in the external adsorption structures (in the magnitude of 0.01 e).

Table S5 The interaction energy between U atoms and CNTs (contained BSSE).

Interaction energy (eV)	U-CNT(12.4 Å)	U-CNT(19.8 Å)
inner	-2.87	-3.03
outer	-2.15	-2.25

To compare the interaction strength of the two systems, we also calculated the interaction energy E_{int}, defined as E_{int}= E(U-CNT) − E(U) − E(CNT), where E(U-CNT) is the total energy of the U-CNT system, while E(U) and E(CNT) denote the total energies of the U fragment and the CNT fragment, respectively, with both the U atom and CNT being in the same atomic configurations as in the relaxed U-CNT system. The basis set superposition errors (BSSE) corrections have been considered during these E_{int} calculations. From Table S5, the results show that with increase of the CNT length, the interaction energies between U atoms and internal / external surfaces of CNT also increased (in the magnitude of 0.1 eV). Also, for the systems of the same length, the interior adsorption is more stable than that of the external one.

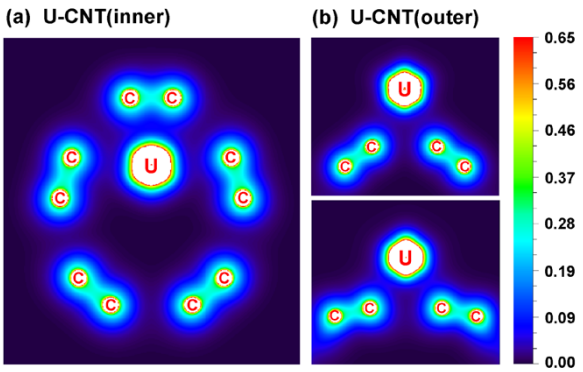

Fig. S3 Electron density distributions of U atoms adsorbed on the 19.8 Å long CNT (inner, a) and (outer, b) systems. The section of (a) is through the U atom and its adsorbed C-C bond; (b) There are two cases of U-CNT(outer) section, the top shows two C atoms that have larger distance among its adsorbed six-ring through U atom, the bottom shows two opposite C atoms among four close atoms in the adsorbed six-ring through U atom (see Fig. S1). The white region in the figure indicates where the electron density is beyond the upper limit of the scale 0.65.

From Fig. S3(a) and (b), it can be seen that in the internal adsorbed U atoms system, there is significant electron accumulation between the U atom and two C atoms on the adsorbed C-C bond, which indicates the presence of valence interactions. For the U atoms adsorbed on the outside of the CNT system, the electron accumulation between the U atom and CNT is not evident; therefore there is almost no covalent interaction.

(4) Orbital

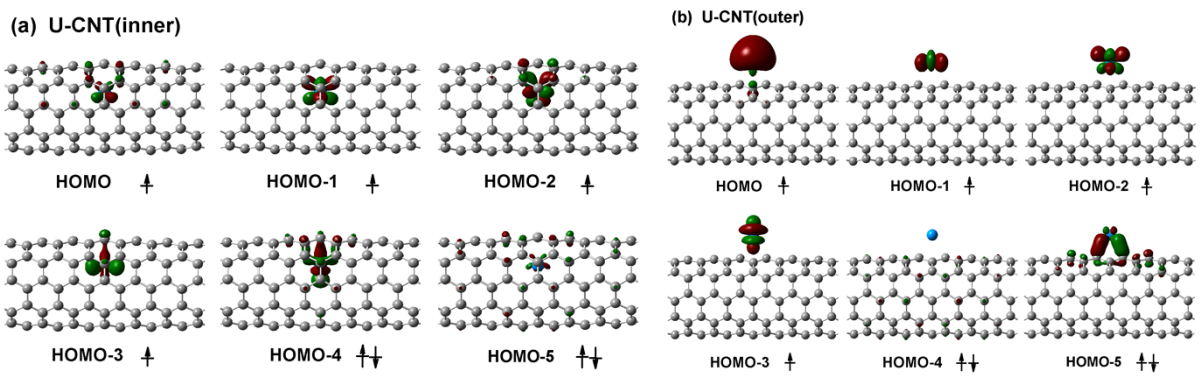

Fig. S4 Frontier molecular orbital of U atoms adsorbed on the 19.8 Å long CNT (inner, a) and (outer, b) systems, in accordance with the order of α electron. In (a), the highest occupied orbital of α electron HOMO-α is the HOMO of the system, and the highest occupied orbital of β electron HOMO-β is the HOMO-4; In (b), the highest occupied molecular orbital of α electron HOMO-α is the HOMO of the system, and the highest occupied orbital of β electron HOMO-β is the HOMO-5. Isovalue = 0.035.

The ground states of both systems are quintet, that is, there are four unpaired electrons. From Fig. S4 and Table S6 we can see that, in the U-CNT (inner) system, the orbitals HOMO ~ HOMO-3 are single occupied. In the HOMO orbital, the U atom's contribution is about 16.07%, and the majority comes from the contribution of CNT. The HOMO-1 orbital is mostly from the contribution of 5f electrons of U atom, which is approximately 91.67%. In the HOMO-2 and HOMO-3 orbitals, the contribution of U atom is 68.01% and 73.78%,

respectively which is still quite large. But they mainly exhibit on the orbital hybridization between the U atom and the adjacent C atoms, which indicates strong covalent interactions between the U and the CNT wall, and is consistent with the previous results about spin and charge distribution. In the U-CNT (outer) system, the single occupied molecular orbitals are HOMO ~ HOMO-3. According to the analysis of orbital component, these four orbitals are mostly from the U atom's contribution, about 78% ~ 99%, while the CNT contributes very little. It is suggested that there is no covalent interaction but electrostatic attraction between the U and the CNT wall.

Table S6 Contribution of U atomic orbitals to the frontier molecular orbitals of the systems of U atoms adsorbed on the 19.8 Å long CNT. (Only the contribution of 5f and 6d electrons of U is listed. In the case that the 5f and 6d electrons' contribution is relatively small, the largest contributor to the orbital is presented and marked with superscripts.)

Orbital composition (%)		HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4	HOMO-5
U-CNT (inner)	Total	16.07	91.67	68.01	73.78	41.85	3.28
	5f	15.25	90.98	64.90	73.51	39.77	2.00
	6d	0.82	0.68	3.10	0.26	1.73	1.24
U-CNT (outer)	Total	78.73	95.13	95.09	98.59	1.03	25.72
	5f	62.25^{7s}	94.53	90.70	92.07	0.18	16.85
	6d	7.48^{7p}	0.52	2.08	5.27^{7s}	0.80	8.86

(5) Electronic density of states

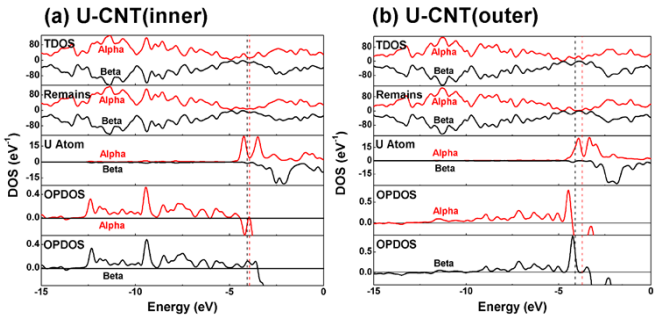

Fig. S5 Distribution of the electronic state density in the U atoms adsorbed on the 19.8 Å long CNT (inner, a) and (outer, b) systems. The red dotted line represents the HOMO-α position, and the black dashed line indicates the HOMO-β position. FWHM = 0.01.

Fig. S5 shows the electronic density of states of U-CNT(inner) and U-CNT(outer) systems. According to the analysis of total DOS and PDOS of U atom, the peaks near the red and black lines exhibit the significant characteristics of the U atom's contribution. Consistent with the orbital analysis (Fig. S4), the frontier molecular orbital of the two systems are mainly contributed by the U atoms. As can be seen in Fig. S5, for the U-CNT(inner) system, the highest occupied molecular orbital of Alpha and Beta electron (HOMO-α and HOMO-β correspond to the HOMO and HOMO-4, respectively) are from the contributions of both CNT and U atom; for the U-CNT(outer) system, the HOMO-α (corresponding to the HOMO) is contributed mostly by the U atom, and the HOMO-β (corresponding to the HOMO-5) is mainly contributed by the CNT. These results are in good accordance with the previous orbital analysis. As shown in the Remains part, the difference between Alpha and Beta of U-CNT(inner) system is larger than that of U-CNT(outer). This indicated that in the internal adsorption system, the CNT is more affected by the U atom, even with changed energy level, resulting in a strong bonding effect between them. The interaction between U atoms and the CNT can be directly observed on the OPDOS curve, where the positive values represent the bonding interaction, the negative values indicate the anti-bonding interaction, and 0 is the non-bonding interaction. In the figure, the HOMO-α of U-CNT(inner) system and HOMO-β of both systems are the bonding orbitals, HOMO-α of U-CNT(outer) system is the lone-electron orbital, which coincide well with the orbital chart. It is also noted that, the difference between HOMO-α and HOMO-β in U-CNT(inner) is as small as 0.11 eV, but in the U-CNT(outer) it is 0.36 eV. This difference can be explained by the orbital. The HOMO-α and HOMO-β of U-CNT(inner) system are contributed by both the CNT and U atom, and the U atom's contribution is from the 5f electrons. As comparison, for the U-CNT(outer) system, the HOMO-α is from the contribution of U atom 7s electrons, while the HOMO-β is mainly the contribution of CNT, and the U atom contribution is from its 5f electrons.

All the results above are consistent with the results in the main text, indicating the reliability of the model we applied.

3. Infrared and Raman spectra of U-CNT(inner) and U-CNT(outer) systems

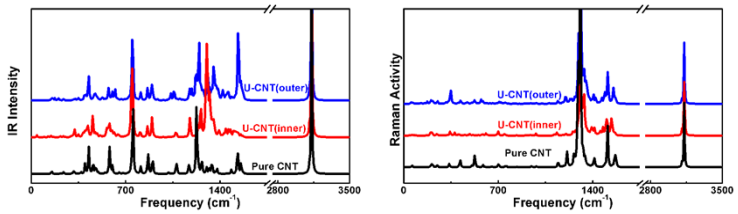

Fig. S6 Infrared and Raman spectra of U-CNT(inner) and U-CNT(outer) systems.

4. The same vibrational mode of pure CNT, U-CNT(inner) and U-CNT(outer).

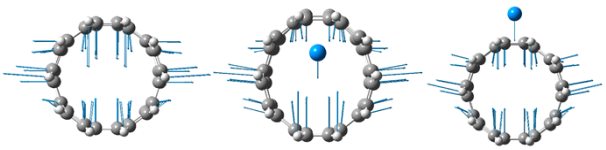

Fig. S7 The same vibrational mode of pure CNT, U-CNT(inner) and U-CNT(outer). When the U atom is adsorbed on the surface of CNT, the vibrational mode of pure CNT at 60.9 cm^{-1} is retained, meanwhile is turned to the cooperative vibration with U participation.

5. Isogram of electronic density distribution of the U-CNT(inner) and U-CNT(outer) systems

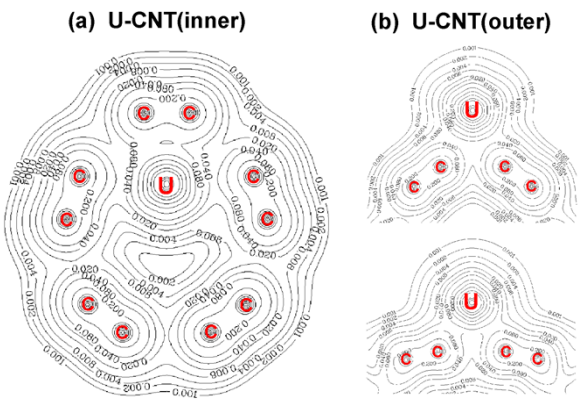

Fig. S8 Isogram of electronic density distribution of the U-CNT(inner) and U-CNT(outer) systems.

6. Curvature effect on the interaction between U atoms and the internal surface of CNTs.

We chose the singlet wall (6, 6), (7, 7), (8, 8) CNTs which have the similar length of about 12.4 Å like the (5, 5) SWCNT in the main text. Using the same BP86/6-31G* method, the structural optimization and electronic states analysis of these U-CNT systems have been performed. The results are summarized in Table S7.

Table S7 Relative energy of the stable adsorption sites of the four adsorption systems. (Select the ground state of each individual system as the zero of energy)

System	Stable adsorption sites	Multiplicity	Relative energy (eV)
U-(5,5)-inner	Bridge	3	0.05
		5	**0**
		7	0.21
U-(6,6)-inner	Bridge	3	0.16
		5	**0**
		7	0.15
U-(7,7)-inner	Hole	3	0.11
		5	**0**
		7	0.21
U-(8,8)-inner	Hole	3	0.26
		5	**0**
		7	0.20

As shown in Table S7, the most stable sites are changed with the decrease of CNTs curvature. For (5, 5) and (6, 6) CNTs, the bridge sites are most stable. By contrast, the most stable sites began to change into hole site from (7, 7) CNT. As the curvature continue to decrease, the most stable adsorption site is maintained at the hole site, such as (8, 8) CNT. Although the decrease of curvature could lead to change of stable adsorption sites of U atoms, ground electronic states of the adsorption systems still remained quintet.

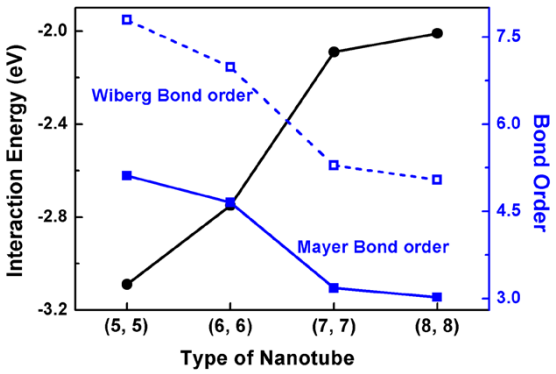

Fig. S9 Interaction energy and bond order between U atoms and adsorbed carbon nanotubes. The black curve denote the interaction energy, the blue dashed and solid curves represent Wiberg and Mayer bond orders respectively.

In order to compare the interaction of the four systems, we calculated the interaction energy E_{int} (contained BSSE). As indicated by the black curve in Fig. S9, the smaller the curvature of CNT is, the weaker the interaction between U atom and CNT becomes. Bond order analysis could directly reflect the strength of bonding between the two fragments of adsorption systems. The blue dashed and solid curves in Fig. S9 denote the Wiberg and Mayer bond order respectively. Although they are different in numerical values, the trends are the same, it means that with the decreasing curvature of CNTs, the bond order between the U atom and the internal surface of CNTs also decreased (i.e. the interaction weakens gradually).

7. Coordinates of the ground state structures in the main text

U-CNT(inner)

C	2.55618500	2.54519000	4.96727200
C	1.93013400	3.03997300	6.16431900
C	2.56975700	2.51148800	0.00000000
C	1.94792200	2.88938900	1.23940900
C	2.54478000	2.49929100	2.48680200
C	0.54229600	3.28427800	3.72383600
C	1.93467600	2.89822800	3.72722800
C	-0.18306300	3.34293700	4.95835900
C	0.60342700	3.42945000	6.15927600
C	2.55618500	2.54519000	-4.96727200
C	1.93467600	2.89822800	-3.72722800
C	2.54478000	2.49929100	-2.48680200
C	0.56120400	3.23561900	-1.23888000
C	1.94792200	2.88938900	-1.23940900
C	-0.15590900	3.19469400	0.00000000
C	0.56120400	3.23561900	1.23888000
C	-1.53699200	2.80946800	2.48765700
C	-0.17147700	3.22855800	2.48027900
C	-2.16489300	2.49320400	3.74136300
C	-1.57555900	2.94030800	4.96415500
C	-3.11741100	1.49956900	6.20893600
C	-2.26542600	2.58290200	6.18246600
C	0.60342700	3.42945000	-6.15927600
C	1.93013400	3.03997300	-6.16431900
C	-0.18306300	3.34293700	-4.95835900
C	0.54229600	3.28427800	-3.72383600
C	-1.53699200	2.80946800	-2.48765700
C	-0.17147700	3.22855800	-2.48027900
C	-2.15296600	2.39325200	-1.24826800
C	-1.52994900	2.76825600	0.00000000
C	-3.16529100	1.37027100	1.25651600

	C	-2.15296600	2.39325200	1.24826800
	C	-3.41094600	0.71606800	2.54156800
	C	-3.11402500	1.39362100	3.76431000
	C	-3.35095300	-0.71657100	5.01373400
5	C	-3.34914700	0.72448400	5.01364900
	C	-3.12087200	-1.49201300	6.20912900
	C	-2.26542600	2.58290200	-6.18246600
	C	-1.57555900	2.94030800	-4.96415500
	C	-3.11402500	1.39362100	-3.76431000
10	C	-2.16489300	2.49320400	-3.74136300
	C	-3.41094600	0.71606800	-2.54156800
	C	-3.16529100	1.37027100	-1.25651600
	C	-3.57528300	-0.72844200	0.00000000
	C	-3.57284800	0.73637600	0.00000000
15	C	-3.16945300	-1.36350400	1.25667700
	C	-3.41305400	-0.70839500	2.54166200
	C	-2.17110400	-2.48828400	3.74154300
	C	-3.11772300	-1.38650800	3.76448800
	C	-1.58250300	-2.93643900	4.96434200
20	C	-2.27139500	-2.57730300	6.18270900
	C	-3.11741100	1.49956900	-6.20893600
	C	-3.35095300	-0.71657100	-5.01373400
	C	-3.34914700	0.72448400	-5.01364900
	C	-3.11772300	-1.38650800	-3.76448800
25	C	-3.41305400	-0.70839500	-2.54166200
	C	-2.15943100	-2.38874500	-1.24836800
	C	-3.16945300	-1.36350400	-1.25667700
	C	-1.53742700	-2.76542800	0.00000000
	C	-2.15943100	-2.38874500	1.24836800
30	C	-0.17930200	-3.22751400	2.48037300
	C	-1.54404600	-2.80601000	2.48782700
	C	0.53446400	-3.28482100	3.72382600
	C	-0.19092000	-3.34202100	4.95842600
	C	1.92303100	-3.04375800	6.16425900
35	C	0.59550900	-3.43037000	6.15928400
	C	-2.27139500	-2.57730300	-6.18270900
	C	-3.12087200	-1.49201300	-6.20912900
	C	-1.58250300	-2.93643900	-4.96434200
	C	-2.17110400	-2.48828400	-3.74154300
40	C	-0.17930200	-3.22751400	-2.48037300
	C	-1.54404600	-2.80601000	-2.48782700
	C	0.55329500	-3.23578400	-1.23884500
	C	-0.16382300	-3.19355000	0.00000000
	C	1.94073000	-2.89255600	1.23936600
45	C	0.55329500	-3.23578400	1.23884500
	C	2.53860100	-2.50402400	2.48677400
	C	1.92768000	-2.90171400	3.72717400
	C	3.45647800	-1.41884500	4.97262200
	C	2.55006900	-2.55018500	4.96719700
50	C	3.76829700	-0.69462100	6.17769100
	C	0.59550900	-3.43037000	-6.15928400
	C	-0.19092000	-3.34202100	-4.95842600
	C	1.92768000	-2.90171400	-3.72717400
	C	0.53446400	-3.28482100	-3.72382600
55	C	2.53860100	-2.50402400	-2.48677400
	C	1.94073000	-2.89255600	-1.23936600
	C	3.46966700	-1.40408600	0.00000000
	C	2.56356100	-2.51623100	0.00000000
	C	3.70429700	-0.72014500	1.24405300
60	C	3.44149500	-1.39751400	2.48855700
	C	3.67688900	0.71790100	3.73881400
	C	3.67508900	-0.72546900	3.73879800
	C	3.45999000	1.41174300	4.97266700
	C	3.77000400	0.68670000	6.17770800
65	C	1.92303100	-3.04375800	-6.16425900
	C	3.45647800	-1.41884500	-4.97262200
	C	2.55006900	-2.55018500	-4.96719700
	C	3.67508900	-0.72546900	-3.73879800
	C	3.44149500	-1.39751400	-2.48855700
70	C	3.70607000	0.71260300	-1.24406400
	C	3.70429700	-0.72014500	-1.24405300

C	3.47315500	1.39714900	0.00000000
C	3.70607000	0.71260300	1.24406400
C	3.44498900	1.39058600	2.48858500
C	3.77000400	0.68670000	-6.17770800
C	3.76829700	-0.69462100	-6.17769100
C	3.45999000	1.41174300	-4.97266700
C	3.67688900	0.71790100	-3.73881400
C	3.44498900	1.39058600	-2.48858500
U	-1.28895900	-0.00034700	0.00000000
H	0.11173900	-3.66972200	-7.11188500
H	-2.01150900	-3.07349500	-7.12349500
H	-3.50794700	-1.13858000	-7.17091300
H	-3.50545400	1.14721900	-7.17072800
H	-2.00458000	3.07867000	-7.12321100
H	0.12009300	3.66962500	-7.11189000
H	2.45899700	2.97664600	-7.12122800
H	3.85050800	1.21839800	-7.13179500
H	3.84748500	-1.22654800	-7.13176000
H	2.45216200	-2.98178800	-7.12110900
H	-3.50794700	-1.13858000	7.17091300
H	-3.50545400	1.14721900	7.17072800
H	-2.00458000	3.07867000	7.12321100
H	0.12009300	3.66962500	7.11189000
H	2.45899700	2.97664600	7.12122800
H	3.85050800	1.21839800	7.13179500
H	3.84748500	-1.22654800	7.13176000
H	2.45216200	-2.98178800	7.12110900
H	0.11173900	-3.66972200	7.11188500
H	-2.01150900	-3.07349500	7.12349500

U-CNT(outer)

C	4.96453700	0.72513000	-4.11830100
C	6.16751500	1.49261000	-3.92873400
C	0.00000000	0.72011400	-4.08997200
C	1.23847000	1.40318900	-3.85479400
C	2.48290100	0.71298600	-4.07148900
C	3.72971600	2.55414900	-2.99017700
C	3.72947300	1.39631100	-3.85289200
C	4.96399800	3.00556900	-2.42595900
C	6.16707200	2.60154300	-3.10482300
C	-4.96453700	0.72513000	-4.11830100
C	-3.72947300	1.39631100	-3.85289200
C	-2.48290100	0.71298600	-4.07148900
C	-1.23852400	2.54974700	-2.99650800
C	-1.23847000	1.40318900	-3.85479400
C	0.00000000	2.97141800	-2.41061400
C	1.23852400	2.54974700	-2.99650800
C	2.48357400	3.37719700	-1.03695400
C	2.48265300	2.95886300	-2.39914500
C	3.72913300	3.38805400	-0.32000300
C	4.96457900	3.44066500	-1.04177900
C	6.16856100	3.09179300	1.06174600
C	6.16647100	3.51155000	-0.25582200
C	-6.16707200	2.60154300	-3.10482300
C	-6.16751500	1.49261000	-3.92873400
C	-4.96399800	3.00556900	-2.42595900
C	-3.72971600	2.55414900	-2.99017700
C	-2.48357400	3.37719700	-1.03695400
C	-2.48265300	2.95886300	-2.39914500
C	-1.23925600	3.37738100	-0.31255800
C	0.00000000	3.38934300	-1.03329200
C	1.24102700	2.93280900	1.04588900
C	1.23925600	3.37738100	-0.31255800
C	2.48942000	2.51662700	1.63997600
C	3.73265600	2.94675300	1.05425600
C	4.97184100	1.41778500	2.53843900
C	4.96944100	2.58001900	1.66784200
C	6.18305300	0.68921000	2.82821800
C	-6.16647100	3.51155000	-0.25582200
C	-4.96457900	3.44066500	-1.04177900
C	-3.73265600	2.94675300	1.05425600

	C	-3.72913300	3.38805400	-0.32000300
	C	-2.48942000	2.51662700	1.63997600
	C	-1.24102700	2.93280900	1.04588900
	C	0.00000000	1.39298400	2.50939000
5	C	0.00000000	2.53720200	1.64303300
	C	1.24386300	0.76077800	2.86936200
	C	2.49493500	1.40551700	2.52711800
	C	3.74355700	-0.72794800	2.76103600
	C	3.74355700	0.72794800	2.76103600
10	C	4.97184100	-1.41778500	2.53843900
	C	6.18305300	-0.68921000	2.82821800
	C	-6.16856100	3.09179300	1.06174600
	C	-4.97184100	1.41778500	2.53843900
	C	-4.96944100	2.58001900	1.66784200
15	C	-3.74355700	0.72794800	2.76103600
	C	-2.49493500	1.40551700	2.52711800
	C	-1.24386300	-0.76077800	2.86936200
	C	-1.24386300	0.76077800	2.86936200
	C	0.00000000	-1.39298400	2.50939000
20	C	1.24386300	-0.76077800	2.86936200
	C	2.48942000	-2.51662700	1.63997600
	C	2.49493500	-1.40551700	2.52711800
	C	3.73265600	-2.94675300	1.05425600
	C	4.96944100	-2.58001900	1.66784200
25	C	6.16647100	-3.51155000	-0.25582200
	C	6.16856100	-3.09179300	1.06174600
	C	-6.18305300	-0.68921000	2.82821800
	C	-6.18305300	0.68921000	2.82821800
	C	-4.97184100	-1.41778500	2.53843900
30	C	-3.74355700	-0.72794800	2.76103600
	C	-2.48942000	-2.51662700	1.63997600
	C	-2.49493500	-1.40551700	2.52711800
	C	-1.24102700	-2.93280900	1.04588900
	C	0.00000000	-2.53720200	1.64303300
35	C	1.23925600	-3.37738100	-0.31255800
	C	1.24102700	-2.93280900	1.04588900
	C	2.48357400	-3.37719700	-1.03695400
	C	3.72913300	-3.38805400	-0.32000300
	C	4.96399800	-3.00556900	-2.42595900
40	C	4.96457900	-3.44066500	-1.04177900
	C	6.16707200	-2.60154300	-3.10482300
	C	-6.16856100	-3.09179300	1.06174600
	C	-4.96944100	-2.58001900	1.66784200
	C	-3.72913300	-3.38805400	-0.32000300
45	C	-3.73265600	-2.94675300	1.05425600
	C	-2.48357400	-3.37719700	-1.03695400
	C	-1.23925600	-3.37738100	-0.31255800
	C	0.00000000	-2.97141800	-2.41061400
	C	0.00000000	-3.38934300	-1.03329200
50	C	1.23852400	-2.54974700	-2.99650800
	C	2.48265300	-2.95886300	-2.39914500
	C	3.72947300	-1.39631100	-3.85289200
	C	3.72971600	-2.55414900	-2.99017700
	C	4.96453700	-0.72513000	-4.11830100
55	C	6.16751500	-1.49261000	-3.92873400
	C	-6.16647100	-3.51155000	-0.25582200
	C	-4.96399800	-3.00556900	-2.42595900
	C	-4.96457900	-3.44066500	-1.04177900
	C	-3.72971600	-2.55414900	-2.99017700
60	C	-2.48265300	-2.95886300	-2.39914500
	C	-1.23847000	-1.40318900	-3.85479400
	C	-1.23852400	-2.54974700	-2.99650800
	C	0.00000000	-0.72011400	-4.08997200
	C	1.23847000	-1.40318900	-3.85479400
65	C	2.48290100	-0.71298600	-4.07148900
	C	-6.16751500	-1.49261000	-3.92873400
	C	-6.16707200	-2.60154300	-3.10482300
	C	-4.96453700	-0.72513000	-4.11830100
	C	-3.72947300	-1.39631100	-3.85289200
70	C	-2.48290100	-0.71298600	-4.07148900
	U	0.00000000	0.00000000	4.95011100

	H	-7.12398500	-3.01689400	1.59188200
	H	-7.13697000	-1.22207700	2.90143900
	H	-7.13697000	1.22207700	2.90143900
	H	-7.12398500	3.01689400	1.59188200
	H	-7.12003900	3.75535300	-0.73589300
	H	7.12003900	3.75535300	-0.73589300
	H	7.12398500	3.01689400	1.59188200
	H	7.13697000	1.22207700	2.90143900
	H	7.13697000	-1.22207700	2.90143900
	H	7.12398500	-3.01689400	1.59188200
	H	7.12003900	-3.75535300	-0.73589300
	H	7.12128500	-3.07827700	-2.85667600
	H	7.12191000	-1.11692600	-4.31261600
	H	7.12191000	1.11692600	-4.31261600
	H	7.12128500	3.07827700	-2.85667600
	H	-7.12128500	3.07827700	-2.85667600
	H	-7.12191000	1.11692600	-4.31261600
	H	-7.12191000	-1.11692600	-4.31261600
	H	-7.12128500	-3.07827700	-2.85667600
	H	-7.12003900	-3.75535300	-0.73589300