CHIN. PHYS. LETT. Vol. 36, No. 11 (2019) 116401 **Express Letter**

Magnetic Coupling Induced Self-Assembly at Atomic Level *

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Developing accurate self-assembly is the key for constructing functional materials from a bottom-up approach. At present, it is mainly hindered by building blocks and driving modes. We design a new self-assembly method based on the magnetic coupling between spin-polarized electrons. First-principles calculations show that spin-polarized electrons from different endohedral metallofullerene (EMF) superatoms can pair each other to ensure a one-dimensional extending morphology. Furthermore, without ligand passivation, the EMF superatoms maintain their electronic structures robustly in self-assembly owing to the core-shell structure and the atomic-like electron arrangement rule. Therefore, it should noted that the magnetic coupling of monomeric electron spin polarization can be an important driving mechanism for high-precision self-assembly. These results represent a new paradigm for self-assembly and offer fresh opportunities for functional material construction at the atomic level.

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Self-assembly, a scientific issue that has garnered much interest,[1,2] is a widely applied strategy in chemical and material science for designing artificial structures from simple building blocks.[3–5] Realizing accurate self-assembly at the atomic level is the ultimate goal, however, huge challenges remain. For instance, it is still difficult to control the morphology and the electronic states in a self-assembly process. Further, traditional self-assembly methods have their own limitations, such as often destroying the stability of the building block itself and requiring very complex ligand structures.[6–9] In fact, during the self-assembly process, it is difficult or even contradictory for building blocks to have strong bond strengths without destroying their structures. In addition, the traditional self-assembly methods are usually regulated by thermal diffusion, which often leads to uncertainty. Therefore, it is particularly important to realize atomic-level control rather than relying on thermal motion.

Achieving controllable self-assembly of both morphology and electronic state has always been a subject of interest.[10] Its success depends on many factors, such as building block structure and interaction, which provides a forward direction for designing the system at the atomic level. Consequently, we can use more stable building blocks of atomic-level precision, e.g., superatom clusters. Such superatom clusters always show extraordinary stability with electronic closed-shell structures.[11–13] Then, if the driving method can be controlled at the atomic level, such as electronic or magnetic recognition effects, we may break the traditional limitations imposed by thermally regulated self-assembly processes.

In this Letter, a new atomic-level self-assembly method, which is driven by magnetic coupling between the building blocks, is presented. Unlike the previous reports, these building blocks can be recognized and combined spontaneously, by means of their own magnetism, and can form stable one-dimensional (1D) chains. Moreover, further analyses indicate that the building blocks can clearly maintain robust structures and have strong bond strengths during the assembly process. Predictably, this approach will lead to the development of atomic-level self-assembly.

To achieve this thought, we employed endohedral metallofullerene (EMF) superatoms U@C_{28} (uranium embedded in C_{28} fullerene) as the building blocks[14] U@C_{28} exhibits the following electronic structural properties: the cage adopts the 32-electron principle using the bonding *s*-, *p*-, *d*-, and *f*-type orbitals of uranium. The remaining two spin polarized electrons cannot break the strong U-cage interactions caused by the 32-electron principle.[15] Subsequently, a series of superatom-assembled structures $(U@C_{28})_n$ ($n = 2$–7) were studied based on first-principles calculations. Despite the existence of multiple assembly structures, we found that the 1D chain was the most stable for each $(U@C_{28})_n$ structure (Fig. S1 and Table S1 in the Supplementary Material). While investigating the reason for the stability of the 1D chains, it was found that a spin-matching phenomenon occurred among the building blocks. Some spin-polarized electrons would flip their spin directions and chemical bonds were formed between the superatoms.[16] Because of the number of spin-polarized electrons in U@C_{28}, only two bonds could be formed, enforcing a chained-link

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configuration. From the spin density analysis, the net spin electrons of these structures were all located at the chain ends. This demonstrates the extensibility of these self-assembly structures and further indicates that the self-assembly process is a local behavior. Thus, the magnetic coupling is a cooperative effect here, including spin flip bonding and spin polarization.

The interaction energies between the building blocks (Fig. 1) decrease gradually as the number of building blocks increases, and this trend is approximately linear. The large interaction energies of these structures show the good thermal stability. These illustrate that the electronic structure of the building blocks is not destroyed. In fact, the reason is that the spin-polarized electrons in $U@C_{28}$ only flip their spin directions during this process, which ensures that this self-assembly process is only a local effect. Furthermore, the inset of Fig. 1 exhibits that the interaction energy curve has a deep potential well in the ES position, which shows the strong bond strength of the assembly structure. The interaction energies between the building blocks were also investigated using energy decomposition analysis (EDA). Orbital interaction contributed more than 70% of the attracting interaction, therefore, the building blocks were connected by strong covalent bonds.

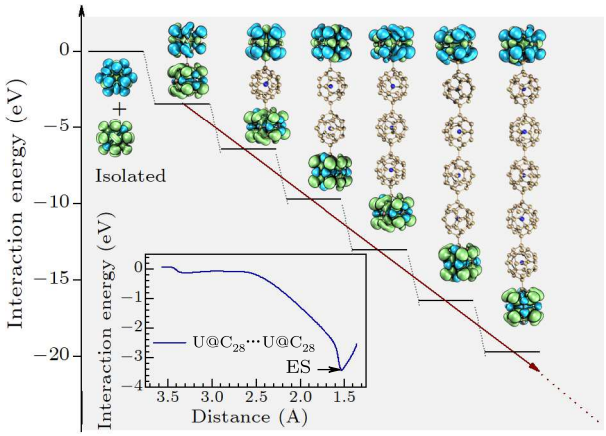

Fig. 1. Interaction energies between the building blocks of $(U@C_{28})_n$ (n = 2–7). The black lines represent the trend of the interaction energies from two isolated $U@C_{28}$ to the equilibrium structures $(U@C_{28})_n$. The brown line was fitted to show the interaction energy more intuitively. The inset image exhibits the interaction energy during the self-assembly of $(U@C_{28})_2$ in detail, and other structures indicate the same change process. The distance represents the bond length between nearest C atoms on different built blocks. ES refers to the equilibrium structure. The isosurface value of the spin density diagram is 0.0005.

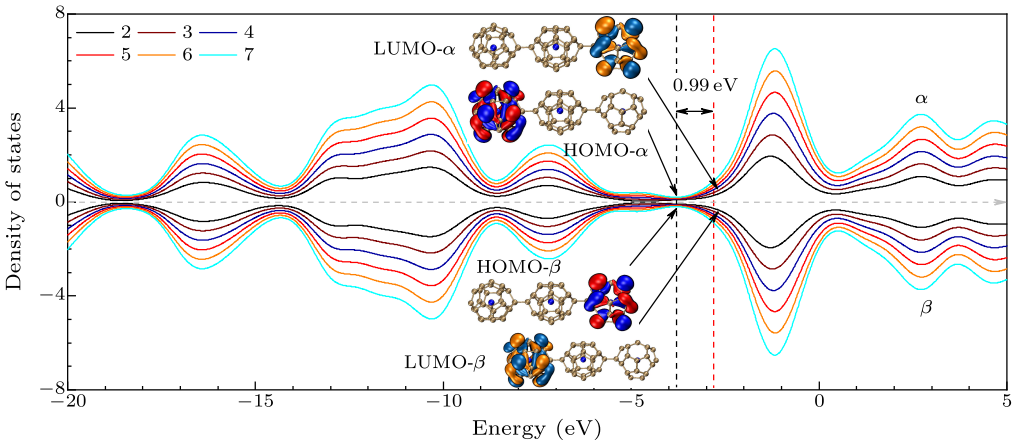

Fig. 2. Density of states of $(U@C_{28})_n$ (n = 2–7). The black and red dotted lines indicate the locations of HOMO and LUMO of $(U@C_{28})_n$, respectively. The isosurface value of the frontier molecular orbital (MO) diagrams is 0.02. Other frontier MO diagrams can be found in Fig. S2 in the Supplementary Material.

According to the above analyses, the structure of the building blocks is still robust under the action of strong bonding, which breaks the limitation of ligand passivation self-assembly. Therefore, unlike the previous chain assembly scheme, EMF building blocks can be assembled by magnetic coupling, which ensures that the structure is not destroyed. Obviously, it is closer to the self-assembly in nature. And for EMFs, there have been successful preparing methods, such as the electrochemical deposition technique for $Sc@C_{82}$ nanowire and tube,[17] liquid-liquid interfacial precipitation (LLIP) technique for $Sc_3N@C_{80}$ nanorods and three-dimensional (3D) nanostructures.[18–19] Furthermore, the aforementioned structures do not require ligand passivation, which highlights the feasibility of magnetic coupling assembly.

To further understand the collective properties of these chains, the following analyses were conducted. First, the density of states (DOS) was plotted (Fig. 2). The results indicated that the highest occupied molecular orbital-lowest unoccupied molecular orbital (HOMO-LUMO) gap of these chains was 0.99 eV. The trends of these DOSs were identical, which showed that the electronic structures do not

change with the increase of the number of building blocks. Overall, these DOS diagrams showed a superimposed property related to the number of building blocks, which revealed that the properties of superatoms can be maintained. The HOMO and LUMO for every chain were located at the chain ends, suggesting that the end building blocks have the highest reactivity. Interestingly, these results revealed that this self-assembly process resembles that of free-radical polymerization.[20] In these chains, there are two electronic states of near-identical energies (Tables S2 and S3 in the Supplementary Material), the low-spin broken-symmetry state and the high-spin triplet state, corresponding to antiferromagnetic coupling and ferromagnetic coupling, respectively.[16] In addition, spin-orbit coupling (SOC) was considered, owing to the existence of low-spin electronic states. The results showed that the frontier molecule orbital energy level splitting was very small (Figs. S3 and S4, Table S4 in the Supplementary Material), demonstrating that the SOC does not significantly impact the properties of the electronic structure.

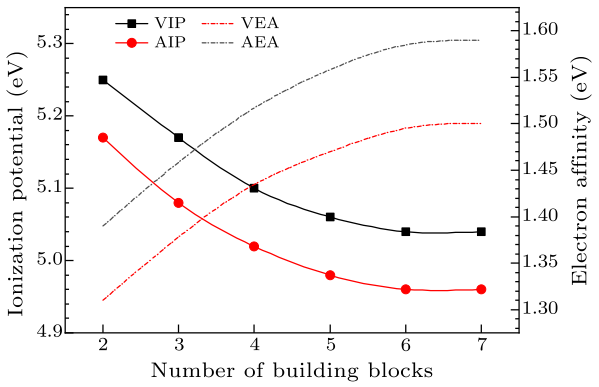

Fig. 3. Redox activity of $(U@C_{28})_n$ (n = 2–7). The abscissa represents the number of building blocks in these chains. VIP: vertical ionization potential, VEA: vertical electron affinity, AIP: adiabatic ionization potential, AEA: adiabatic electron affinity (Table S5 in the Supplementary Material for details).

To measure redox activity in these chains, the ionization potential and electron affinity were analyzed (Fig. 3). With the increase of the number of building blocks, the ionization potential gradually decreased, while the electron affinities increased. It shows that these systems tend to lose electrons, suggesting an enhancement of reducibility. It is worth noting that when $n \geq 6$ for $(U@C_{28})_n$, the electron affinity and ionization potential will not change anymore. Therefore, the redox properties of the chains remain unchanged as the number of building blocks continues to increase. This analysis proves the reliability of this assembly method.

A new accurate self-assembly method is reported via the first-principles DFT calculations. During the self-assembly process, the building blocks tend to be chained and the driving method is magnetic coupling. The interaction energy analyzing indicates that the building blocks have strong bond strengths. The DOS and HOMO-LUMO gap analyses demonstrate that the properties of these chains are not dependent on the number of building blocks. Then, when the building blocks are increased to a certain number, the redox properties of the system will not change anymore. All the above results prove the feasibility of this magnetic-coupling-induced self-assembly method and demonstrate that the assembled building blocks is robust. Admittedly, in this study, we employed the selected EMF superatoms, whereas traditional self-assembly building blocks are almost always transition metals. Because of the inherent chemical activity of transition metals, if we want to assemble them, they will often need to be passivated by ligands. However, the method introduced in this work is different, and the reasons are as follows. Firstly, not only do EMF building blocks have thermal stability like fullerenes, but also they can maintain the excellent quantum properties of embedded metals. Secondly, EMF building blocks have stronger bonds compared with those of transition metal building blocks, allowing them to be assembled without relying on ligands. Finally, the driving method is based on magnetic coupling, which implements effective and accurate control at the atomic level. Furthermore, since magnetic fields can be created and controlled, this study shows great potential for future meaningful applications of magnetically controllable self-assemblies.

In conclusion, the 1D morphology-controllable self-assembly method presented in this study has great application value in the fields of optics and electricity because of its directional transmission characteristics.[21] Our work provides an effective method for precisely positioning a 1D morphology. Further, this method is not limited to linear chains. If the basic building block has another number of spin-polarized electrons, the potential for assembling variously shaped systems becomes possible. Since the self-assembly extension mechanism is closely dominated by the electron-spin polarization characteristics of the assembly building blocks, this study highlights how the magnetic effect of electron-spin polarization in physics can be an important driving mechanism for high-precision self-assembly. These findings will open up a new field for better functionalization[2,22] and control of building blocks, such as superatoms.

Data Availability: The data that support the findings of this study are available from the authors upon request.

Competing Interests: The authors declare that there are no competing interests.

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Author Contributions: W. Xie and Y. Zhu contributed equally to this work. Z. Wang conceived this project. Computational details were performed by W. Xie, Y. Zhu and led by Z. Wang. W. Xie, Y. Zhu, J. Wang and Z. Wang acquired and analyzed the data. W. Xie, Y. Zhu, J. Wang, A. Cheng and Z. Wang prepared the manuscript. We warmly thank W. Jiang and Y. Gao for the stimulating discussions. Z. Wang acknowledges the High Performance Computing Center of Jilin University.

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Supplementary Material: Magnetic Coupling Induced Self-Assembly at Atomic Level*

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Text A: Computation details

All the structures were calculated at M06-2X level, which proved to have an advantage in the calculation of intermolecular interaction. [1-2] In terms of the realistic effect, small-core relativistic effective core potentials (RECP) covering 60 core electrons with the (14s13p10d8f6g)/ [10s9p5d4f3g] valence basis set [3] is used for U, while the valence double-ζ with d-polarization basis set 6-31G* [4] is for C. Density functional theory with the third generation empirical dispersion correction (DFT-D3) [5] at Perdew–Burke–Ernzerhof (PBE) [6] level was also adopted throughout this work. Both scalar relativistic and spin–orbit coupling effects have been taken into account through zeroth-order regular approximations (ZORA). A triple-ζ with polarization functions (TZP) Slater basis set was employed, while a [$1s^2$-$4f^{10}$] frozen core for U and full electrons for C atoms. All optimized structures thus obtained were analyzed with vibration frequency calculations at the same level to avoid imaginary frequencies. The HOMO-LUMO gap for these structures was calculated using Heyd-Scuseria-Ernzerhof screened hybrid functional (HSE06), [7] some researches have shown that the HSE06 functional gives a reasonably faithful reproduction of the band gaps for actinide systems when compared with available experimental data. [8-9] All calculations were performed using Gaussian 09 [10] and ADF 2012 [11]. To accurately describe the magnetic coupling, the broken-symmetry (BS) technique was used to obtain the lowest spin state. [12] The magnetic coupling can be described by using Heisenberg-Dirac-van Vleck (HDVV) spin Hamiltonian (SH) [13-14]. The equation is:

$$\hat{H}^{HDVV} = -J\hat{S}_A\hat{S}_B \quad (1)$$

In Equation 1, $\hat{S}_A$ and $\hat{S}_B$ are the total spin operators of magnetic centers A and B, J is the exchange coupling constant. A positive J indicates ferromagnetic coupling between magnetic centers. A negative J indicates antiferromagnetic coupling.

By using spin-projection technique, the equation can be described as:

$$J = 2(E_{BS}-E_{HS})/S^2_{max} \quad (2)$$

In Equation 2, E_{BS} and E_{HS} are the energies of broken-symmetry state and highest spin state, respectively. S_{max} is the value of the maximum spin. Thus, we could analyze the magnetic coupling from the relative energies of different spin states. Basis sets superposition error (BSSE) is defined as:

$$E_{binding} = E_{total} + E_{BSSE} - (E_{M1} + E_{M2} + \ldots\ldots + E_{Mn}) \quad (3)$$

In Equation 3, E_{total} are the total optimized energy of the complex. E_{M1}, E_{M1}, and E_{Mn} are single-point energies for the monomers with their geometries abstracted form the $(U@C_{28})_n$ and using only the monomeric basis sets. The stability of the wavefunctions of all the involved electronic states in this work is calculated using specialized methods [15] in Gaussian 09 package.

Text B: Spin-orbit coupling (SOC) results

In spin-unrestricted SOC-ZORA calculations, each level can be allocated one electron. However, it is not directly related to spin-α or spin-β, but to more general Kramer's symmetry. Therefore, we do not need to discuss the multiplicity in SOC-ZORA calculations. SOC calculations on $(U@C_{28})_n$ (n=2-5) show that the MO energy level is almost no splitting, and the HOMO-LUMO gap is the same as SR-ZORA results, indicating that SOC has no significant effect on the electronic structures of $(U@C_{28})_n$.

Text C: Details for redox activity analysis

The values of vertical ionization potential (VIP), vertical electron affinity (VEA), adiabatic ionization potential (AIP) and adiabatic electron affinity (AEA) are defined as $E_{VIP} = E^+(sp) - E_0(opt)$, $E_{VEA} = E_0(opt) - E^-(sp)$, $E_{AIP} = E^+(opt) - E_0(opt)$ and $E_{AEA} = E_0(opt) - E^-(opt)$. Where $E_0(opt)$ is the total bonding energy of the structures; $E^+(opt)$ and $E^-(opt)$ represent total bonding energies of the cation and the anion on their respective optimized geometries; $E^+(sp)$ and $E^-(sp)$ represent total bonding energies of the cation and the anion in single-point geometries, respectively.

Figure S1. Optimized local-minimum geometries of $(U@C_{28})_n$ during the self-assembly process.

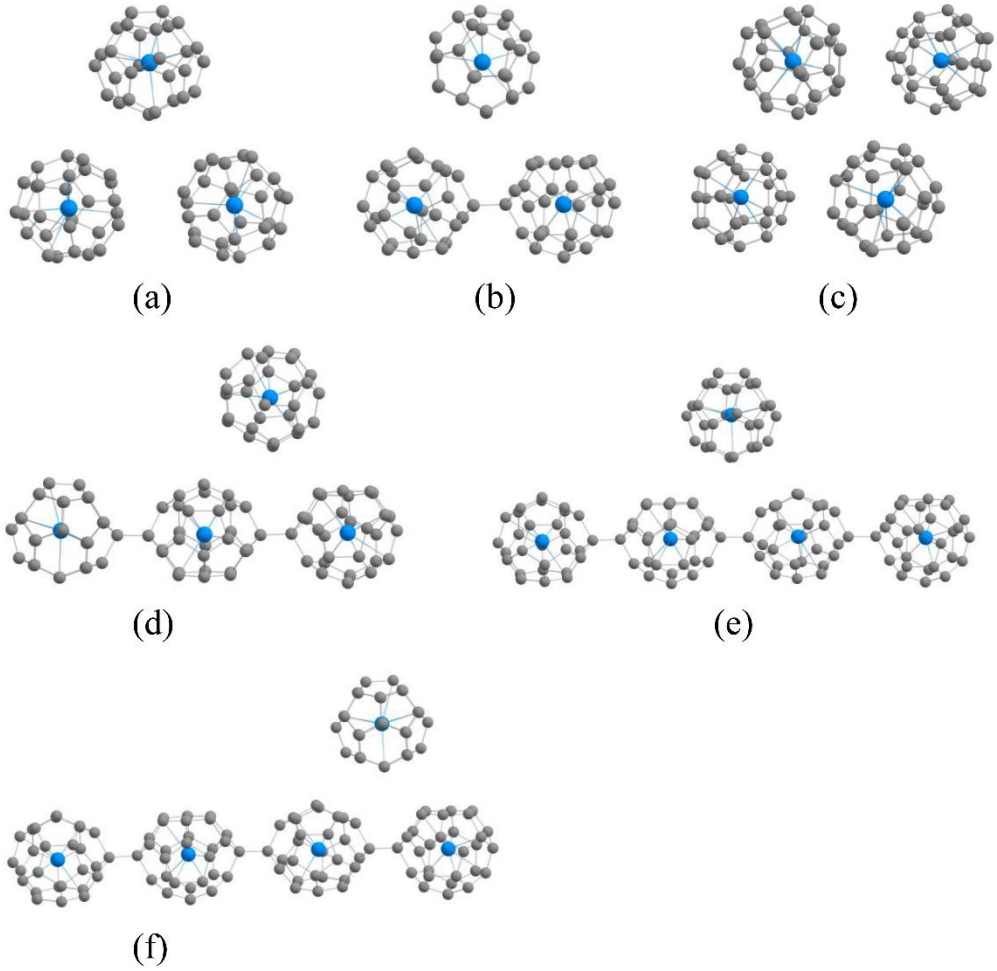

Figure S2. Frontier MOs diagram of $(U@C_{28})_n$. (A), (B), (C), (D) for $(U@C_{28})_2$. (E), (F), (G), (H) for $(U@C_{28})_3$. (I), (J), (K), (L) for $(U@C_{28})_4$. (M), (N), (O), (P) for $(U@C_{28})_5$. (Q), (R), (S), (T) for $(U@C_{28})_6$. (U), (V), (W), (X) for $(U@C_{28})_7$. Isovalue=0.02

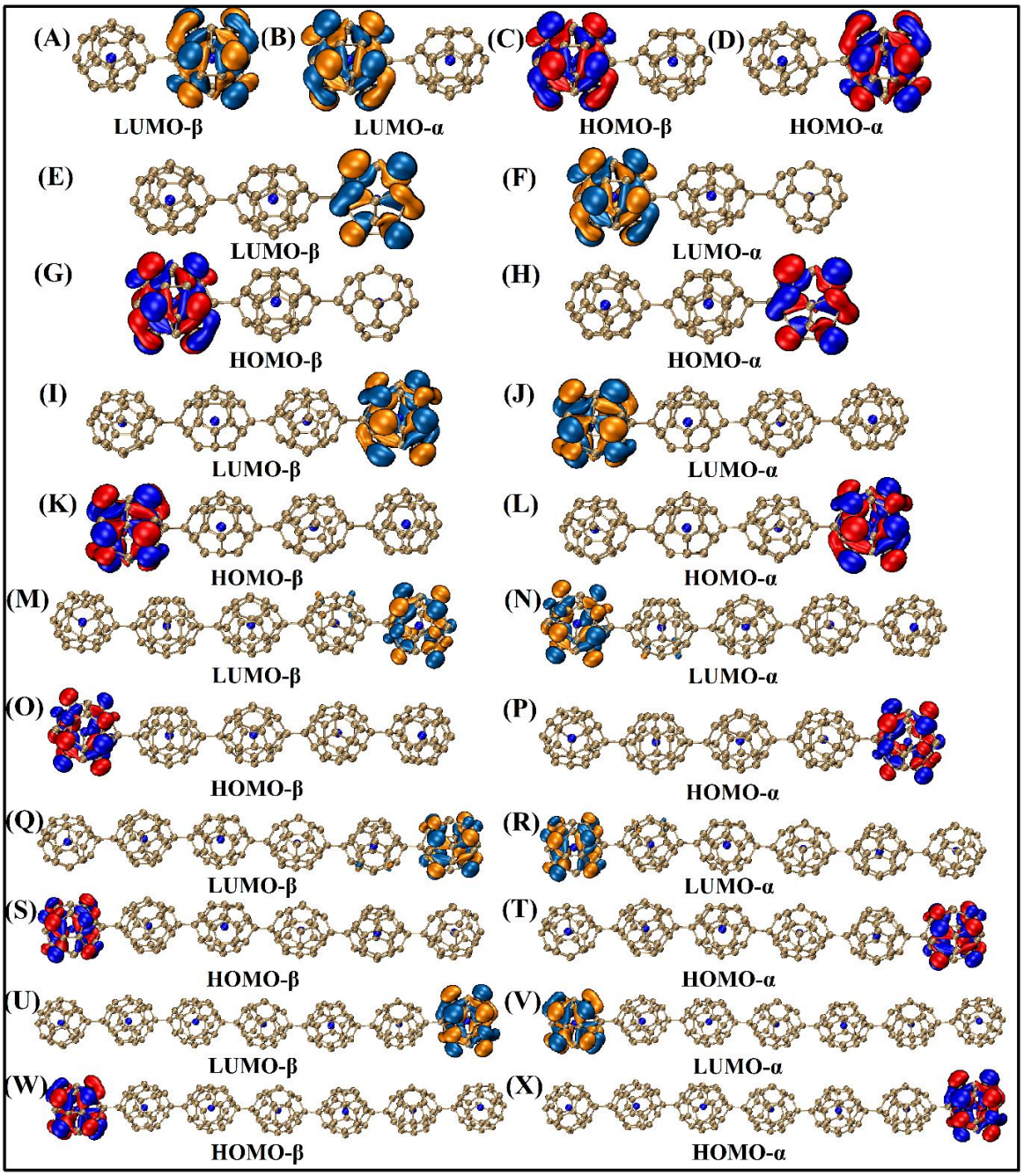

Figure S3. MOs energy levels of $(U@C_{28})_2$ and $(U@C_{28})_3$ MOs including scalar relativistic and spin-orbit coupling effects. Left: PBE-D3 level including scalar relativistic effect. Right: PBE-D3 level including spin-orbit coupling effect. All the irreducible representations of SOC-ZORA MOs (right) are $a_{1/2}$ due to the symmetry was abolished in SOC-ZORA calculations.

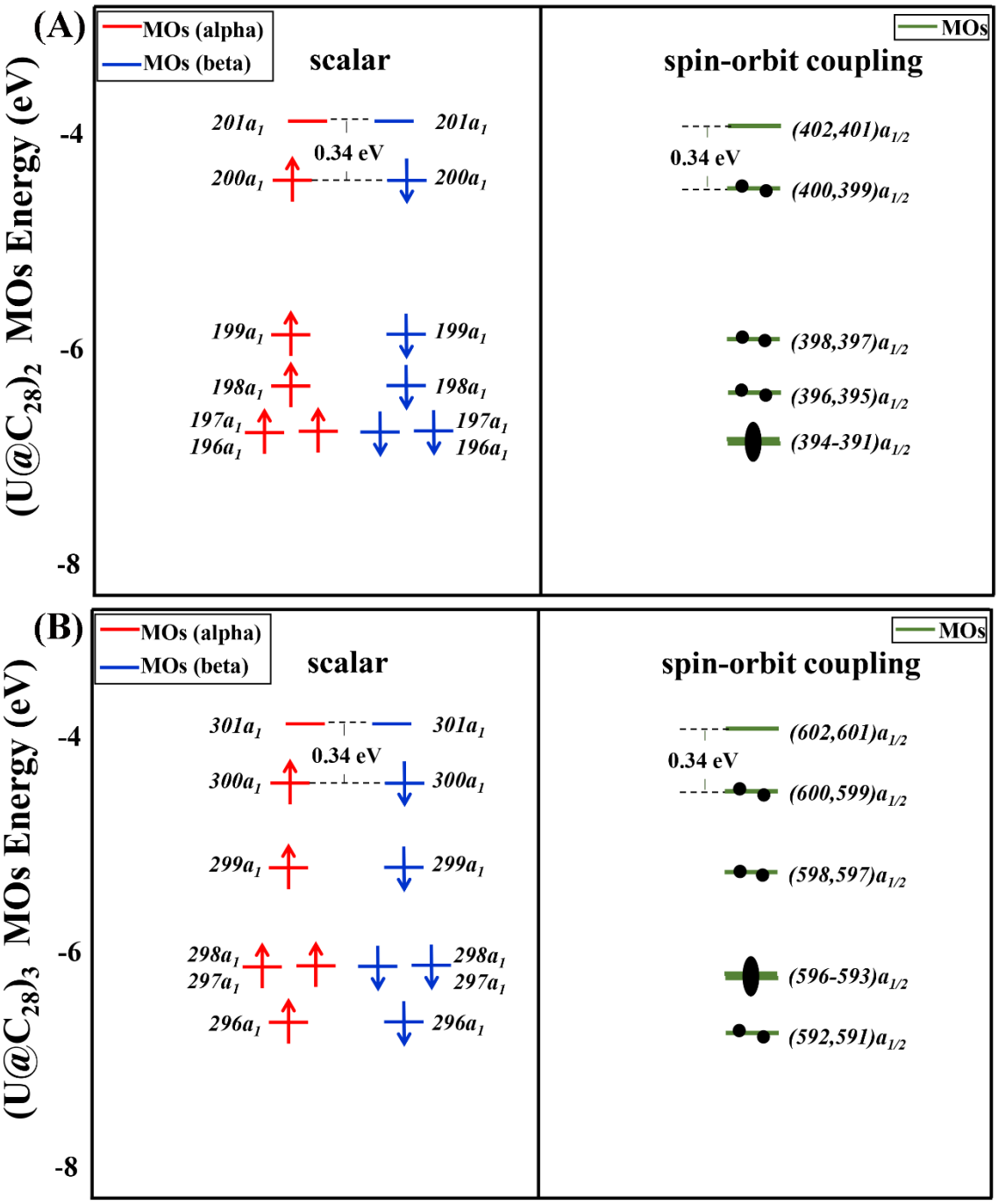

Figure S4. MOs energy levels of $(U@C_{28})_4$ and $(U@C_{28})_5$ MOs including scalar relativistic and spin-orbit coupling effects. Left: PBE-D3 level including scalar relativistic effect. Right: PBE-D3 level including spin-orbit coupling effect. All the irreducible representations of SOC-ZORA MOs (right) are $a_{1/2}$ due to the symmetry was abolished in SOC-ZORA calculations.

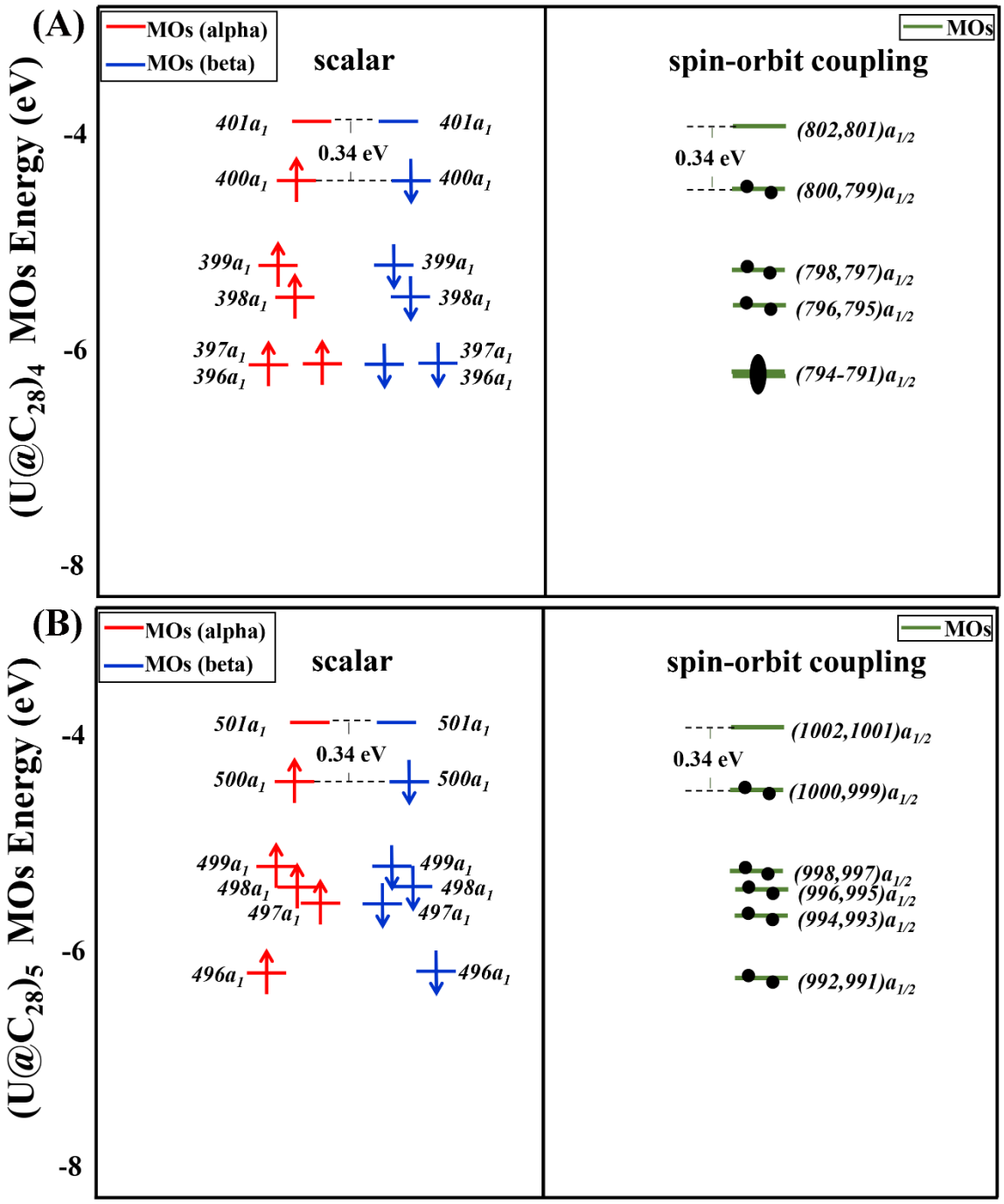

Table S1. Total and relative energies of optimized local-minimum geometries during the self-assembly process using M062x functional of DFT.

	Total Energy (Hartree)	Relative Energies (eV)
(a)	-4628.90429	0
(b)	-4628.99809	-0.093
(c)	-6171.87958	-1542.975
(d)	-6172.04577	-1543.141
(e)	-7715.09373	-3086.189
(f)	-7715.09375	-3086.189

Table S2. Total and relative energies of the different electronic states of $(U@C_{28})_n$ (n=3-5) using M062x functional of DFT.

	El. State	Total energies (Hartree)	Relative Energies (eV)
$(U@C_{28})_3$	BS	-4629.07128	0
	Triplet	-4629.07128	0
	Quintet	-4629.02888	0.042
	Septet	-4628.90450	0.166
$(U@C_{28})_4$	BS	-6172.11929	-1543.048
	Triplet	-6172.11929	-1543.048
	Quintet	-6172.04981	-1542.978
	Septet	-6172.03394	-1542.962
$(U@C_{28})_5$	BS	-7715.16735	-3086.096
	Triplet	-7715.16735	-3086.096
	Quintet	-7715.12514	-3086.053
	Septet	-7715.15532	-3086.084

Table S3. Bond and relative energies of the chained $(U@C_{28})_n$ (n=2-7) in PBE-D3 level including scalar relativistic effect.

	El. State	Bond Energy (eV)	Relative Energies (eV)
$(U@C_{28})_2$	BS	-495.738	0
	Triplet	-495.636	0.102
$(U@C_{28})_3$	BS	-744.535	-248.797
	Triplet	-744.535	-248.797
$(U@C_{28})_4$	BS	-993.325	-497.587
	Triplet	-993.328	-497.590
$(U@C_{28})_5$	BS	-1242.106	-746.368
	Triplet	-1242.107	-746.369
$(U@C_{28})_6$	BS	-1490.954	-995.216
	Triplet	-1490.955	-995.217
$(U@C_{28})_7$	BS	-1739.754	-1244.016
	Triplet	-1739.755	-1244.017

Table S4. Bond and relative energies of the chained $(U@C_{28})_n$ (n=2-5) in PBE-D3 level including spin-orbit coupling effect.

	Bond Energy (eV)	Relative Energies (eV)
$(U@C_{28})_2$	-514.309	0
$(U@C_{28})_3$	-772.407	-258.098
$(U@C_{28})_4$	-1030.511	-516.202
$(U@C_{28})_5$	-1288.577	-774.268

Table S5. Ionization potentials and electron affinities of $(U@C_{28})_n$ (n=2-7). (unit: eV)

	VIP	AIP	VEA	AEA
$(U@C_{28})_2$	5.25	5.17	1.31	1.39
$(U@C_{28})_3$	5.17	5.08	1.38	1.46
$(U@C_{28})_4$	5.10	5.02	1.44	1.52
$(U@C_{28})_5$	5.06	4.98	1.47	1.56
$(U@C_{28})_6$	5.04	4.96	1.50	1.59
$(U@C_{28})_7$	5.04	4.96	1.50	1.59

Table S6. Coordinates of the optimized structures.

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C28)_2$-BS	1	U	-0.003749	3.541620	0.003250
	2	C	-0.755568	5.576050	-1.190100
	3	C	2.470680	3.510840	0.210376
	4	C	-1.025140	3.423510	2.263820
	5	C	-0.734396	1.472810	-1.327060
	6	C	1.173830	2.697630	1.972190
	7	C	-1.820800	3.530990	-1.613300
	8	C	-0.531523	3.562880	-2.370590
	9	C	1.165260	4.202150	2.021710
	10	C	-0.820305	1.431950	1.030680
	11	C	1.456830	4.838910	-1.441340
	12	C	1.343500	5.546890	-0.132320
	13	C	-1.986000	2.192620	0.526299
	14	C	1.367790	1.487320	-0.254014
	15	C	-0.851727	5.492220	1.157210
	16	C	-2.023420	4.752420	0.603070
	17	C	1.466230	2.278270	-1.501190
	18	C	-0.018380	0.767472	-0.139307
	19	C	-2.085770	3.443360	1.270250
	20	C	2.118150	3.548010	-1.199210
	21	C	-0.051100	5.987770	0.026724
	22	C	1.959200	2.280510	0.812926
	23	C	0.137831	2.283660	-2.148850
	24	C	-0.219519	4.645910	2.196070
	25	C	-1.944220	4.791630	-0.868207
	26	C	-0.204760	2.226400	2.084110
	27	C	1.974400	4.700750	0.907255
	28	C	-1.905540	2.233110	-0.948613
	29	C	0.132445	4.843250	-2.088390
	30	U	0.003747	-3.541620	0.003248
	31	C	0.755578	-5.576050	-1.190100
	32	C	1.025140	-3.423510	2.263810
	33	C	0.734387	-1.472810	-1.327050
	34	C	-2.470670	-3.510840	0.210376
	35	C	0.820300	-1.431950	1.030690
	36	C	-1.456820	-4.838920	-1.441350
	37	C	-1.343490	-5.546890	-0.132325
	38	C	1.985990	-2.192610	0.526301
	39	C	-1.367800	-1.487320	-0.254011
	40	C	0.851732	-5.492210	1.157200
	41	C	2.023420	-4.752410	0.603068
	42	C	-1.466230	-2.278280	-1.501190
	43	C	-1.173840	-2.697630	1.972200

	44	C	1.820800	-3.530980	-1.613300
	45	C	0.531527	-3.562880	-2.370590
	46	C	-1.165260	-4.202150	2.021710
	47	C	-1.959210	-2.280510	0.812930
	48	C	-0.137833	-2.283660	-2.148830
	49	C	0.219523	-4.645910	2.196070
	50	C	1.944230	-4.791620	-0.868208
	51	C	0.204756	-2.226400	2.084110
	52	C	-1.974390	-4.700750	0.907253
	53	C	1.905540	-2.233110	-0.948609
	54	C	-0.132437	-4.843250	-2.088390
	55	C	0.018372	-0.767473	-0.139303
	56	C	2.085760	-3.443360	1.270250
	57	C	-2.118150	-3.548020	-1.199210
	58	C	0.051107	-5.987770	0.026721

	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_2$-triplet	1	U	-3.554400	-0.003475	-0.040891
	2	C	-3.483590	-2.239570	1.038010
	3	C	-1.491950	0.238304	-1.544430
	4	C	-3.464770	1.760970	1.704030
	5	C	-5.594590	0.234328	-1.422670
	6	C	-2.240820	2.057030	-0.263305
	7	C	-5.535830	-1.345970	0.316292
	8	C	-4.819290	-1.908060	-0.866141
	9	C	-1.463470	1.160410	0.623430
	10	C	-4.801420	2.075300	-0.203337
	11	C	-2.258910	-1.894160	-0.921832
	12	C	-1.475540	-1.340250	0.206096
	13	C	-5.525190	1.166780	0.734410
	14	C	-3.565620	1.114470	-2.201450
	15	C	-2.701610	-0.383995	2.217810
	16	C	-4.206570	-0.384478	2.262500
	17	C	-3.571760	-0.361232	-2.447400
	18	C	-4.831340	1.473200	-1.548310
	19	C	-4.672770	0.962446	1.928420
	20	C	-2.284150	-0.883604	-1.999710
	21	C	-2.265160	-1.524290	1.415510
	22	C	-2.272700	1.455130	-1.612700
	23	C	-4.842750	-0.903072	-1.944790
	24	C	-2.253590	0.951393	1.829010
	25	C	-4.685870	-1.548800	1.512480
	26	C	-3.496310	2.395160	0.395985
	27	C	-0.777914	0.005859	-0.181431
	28	C	-6.000500	0.004869	-0.034040
	29	C	-3.519360	-2.415790	-0.404526
	30	U	3.554370	0.003554	-0.039354

	31	C	3.463820	-1.771150	1.695140
	32	C	5.595050	-0.226563	-1.421840
	33	C	3.483570	2.233290	1.052660
	34	C	1.492520	-0.229261	-1.545030
	35	C	4.819930	1.912730	-0.852968
	36	C	1.462940	-1.164050	0.617429
	37	C	2.240570	-2.055610	-0.274243
	38	C	5.536050	1.343480	0.326403
	39	C	2.259420	1.899470	-0.909643
	40	C	4.801140	-2.074630	-0.213363
	41	C	5.524640	-1.171800	0.729925
	42	C	1.475640	1.339030	0.214802
	43	C	3.572670	0.375342	-2.443710
	44	C	4.205850	0.370706	2.266530
	45	C	2.700830	0.370833	2.221400
	46	C	3.566310	-1.101710	-2.206460
	47	C	2.284830	0.895284	-1.993660
	48	C	2.264930	1.515970	1.425610
	49	C	4.831790	-1.464490	-1.554970
	50	C	4.672030	-0.974365	1.925000
	51	C	4.843510	0.914071	-1.937500
	52	C	2.273220	-1.445750	-1.620000
	53	C	4.685430	1.539100	1.523490
	54	C	2.252660	-0.962141	1.824370
	55	C	3.519840	2.417690	-0.388890
	56	C	6.000560	-0.005409	-0.031676
	57	C	0.777917	-0.004636	-0.181026
	58	C	3.495730	-2.397900	0.383727

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_3$-BS	1	U	-0.053628	3.666780	-0.218600
	2	C	-0.837915	5.726210	-1.535410
	3	C	2.416210	3.716690	-0.022222
	4	C	-1.095700	3.689320	2.029080
	5	C	-0.759719	1.529480	-1.454830
	6	C	1.128390	2.968190	1.795220
	7	C	-1.864370	3.601340	-1.844540
	8	C	-0.579839	3.610720	-2.595080
	9	C	1.099550	4.484810	1.766380
	10	C	-0.849946	1.613870	0.916190
	11	C	1.379650	4.945630	-1.718450
	12	C	1.272510	5.744460	-0.447257
	13	C	-2.029770	2.358450	0.350338
	14	C	1.349360	1.633200	-0.367848
	15	C	-0.927041	5.728120	0.838276
	16	C	-2.077560	4.920050	0.301818
	17	C	1.427550	2.384790	-1.668670

18	C	-0.033577	0.904807	-0.222001
19	C	-2.143440	3.650760	1.029090
20	C	2.059970	3.682720	-1.426330
21	C	-0.138190	6.423830	-0.326996
22	C	1.902090	2.511600	0.641119
23	C	0.112391	2.353870	-2.276670
24	C	-0.297378	4.909590	1.853190
25	C	-1.960600	4.889080	-1.142340
26	C	-0.251524	2.494420	1.898510
27	C	1.856420	4.925980	0.594986
28	C	-1.912960	2.338790	-1.093740
29	C	0.064615	4.903780	-2.325790
30	U	0.080570	-3.387810	0.117739
31	C	0.894107	-5.456410	-0.974576
32	C	1.070620	-3.145540	2.381500
33	C	0.779787	-1.365870	-1.296480
34	C	-2.396170	-3.407530	0.294038
35	C	0.834857	-1.217210	1.057170
36	C	-1.331210	-4.783710	-1.284450
37	C	-1.218100	-5.429470	0.056197
38	C	2.024090	-1.971570	0.601139
39	C	-1.334660	-1.381070	-0.248162
40	C	0.959084	-5.265200	1.367300
41	C	2.120190	-4.523500	0.793905
42	C	-1.399000	-2.229290	-1.459370
43	C	-1.140820	-2.485840	2.032310
44	C	1.917190	-3.408210	-1.477530
45	C	0.638573	-3.504480	-2.247270
46	C	-1.098030	-3.986200	2.149500
47	C	-1.920980	-2.139630	0.846491
48	C	-0.062825	-2.232830	-2.090800
49	C	0.294565	-4.388510	2.359350
50	C	2.060350	-4.630590	-0.674841
51	C	0.224974	-1.977430	2.138680
52	C	-1.881440	-4.553070	1.049080
53	C	1.963490	-2.080190	-0.871294
54	C	0.000827	-4.785990	-1.915180
55	C	0.032784	-0.625579	-0.150545
56	C	2.143940	-3.184680	1.402050
57	C	-2.025110	-3.499260	-1.108330
58	C	0.184137	-5.829690	0.251237
59	U	0.055748	10.725900	-0.284140
60	C	-1.314840	12.787900	-0.235972
61	C	1.520830	10.601500	1.716470
62	C	-1.501570	8.687370	-0.279126
63	C	1.448650	10.647900	-2.337790
64	C	0.509137	8.621500	0.952819

	65	C	-0.462533	12.013000	-2.279020
	66	C	0.635589	12.708100	-1.545270
	67	C	-0.487549	9.408520	1.712900
	68	C	0.464690	8.650520	-1.583740
	69	C	0.680967	12.679000	1.000970
	70	C	-0.390624	11.967200	1.757230
	71	C	-0.558442	9.453630	-2.289640
	72	C	2.332050	9.838800	-0.334834
	73	C	-2.245210	10.768100	0.505381
	74	C	-2.271660	10.784900	-0.989764
	75	C	2.399290	11.342700	-0.318706
	76	C	1.699370	9.420390	-1.583550
	77	C	-1.774390	9.491100	-1.450580
	78	C	1.879970	11.809700	0.968866
	79	C	-1.632580	12.021800	0.965700
	80	C	1.744160	9.391710	0.925934
	81	C	1.834580	11.838900	-1.575970
	82	C	-1.732380	9.464510	0.918679
	83	C	-1.675680	12.049300	-1.442930
	84	C	-0.129194	7.956600	-0.312772
	85	C	0.135174	10.652000	2.152580
	86	C	0.048306	10.707500	-2.722890
	87	C	0.098513	13.172700	-0.256666

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_3$-triplet	1	U	-0.033088	3.665590	-0.225110
	2	C	-0.828976	5.728940	-1.528730
	3	C	2.439080	3.711500	-0.057027
	4	C	-1.048540	3.686360	2.035170
	5	C	-0.756687	1.532030	-1.456260
	6	C	1.171580	2.961940	1.773980
	7	C	-1.862420	3.606280	-1.829470
	8	C	-0.586582	3.614960	-2.594860
	9	C	1.144830	4.478580	1.748050
	10	C	-0.818931	1.613150	0.915892
	11	C	1.385010	4.945410	-1.738740
	12	C	1.293990	5.742540	-0.465023
	13	C	-2.004300	2.359970	0.365149
	14	C	1.365300	1.629620	-0.393847
	15	C	-0.890016	5.726070	0.845710
	16	C	-2.048450	4.921570	0.321505
	17	C	1.429340	2.384020	-1.694130
	18	C	-0.017251	0.904078	-0.233077
	19	C	-2.107800	3.651280	1.047240
	20	C	2.066430	3.680760	-1.456810
	21	C	-0.114021	6.423380	-0.327285

22	C	1.930730	2.506020	0.610162
23	C	0.107218	2.356340	-2.286820
24	C	-0.250173	4.905340	1.851930
25	C	-1.948290	4.892960	-1.123900
26	C	-0.207751	2.490630	1.892800
27	C	1.888380	4.920590	0.568813
28	C	-1.904320	2.342460	-1.080220
29	C	0.063091	4.906610	-2.330750
30	U	0.064017	-3.387530	0.119380
31	C	0.831718	-5.468480	-0.982330
32	C	1.109040	-3.146490	2.358710
33	C	0.750250	-1.378260	-1.318940
34	C	-2.407600	-3.381680	0.353635
35	C	0.861612	-1.221210	1.032170
36	C	-1.393410	-4.774860	-1.243120
37	C	-1.255430	-5.416240	0.097169
38	C	2.032170	-1.989100	0.551886
39	C	-1.339170	-1.368230	-0.221871
40	C	0.952972	-5.268550	1.356260
41	C	2.107540	-4.540860	0.752982
42	C	-1.439970	-2.220750	-1.427420
43	C	-1.103110	-2.465810	2.058130
44	C	1.862750	-3.432590	-1.517700
45	C	0.565762	-3.519250	-2.257040
46	C	-1.072510	-3.965940	2.180700
47	C	-1.907080	-2.116410	0.889321
48	C	-0.119209	-2.239910	-2.089780
49	C	0.320480	-4.381570	2.359920
50	C	2.012640	-4.653160	-0.713441
51	C	0.269709	-1.970960	2.130640
52	C	-1.886550	-4.529200	1.101360
53	C	1.936070	-2.102910	-0.918158
54	C	-0.076600	-4.792960	-1.904630
55	C	0.037560	-0.626244	-0.158976
56	C	2.158650	-3.200190	1.354870
57	C	-2.070370	-3.482900	-1.056430
58	C	0.146866	-5.829770	0.261105
59	U	0.050395	10.726300	-0.280153
60	C	-1.335340	12.777700	-0.217732
61	C	1.536780	10.613400	1.705570
62	C	-1.490350	8.676110	-0.259418
63	C	1.423380	10.659900	-2.347480
64	C	0.533074	8.625270	0.952323
65	C	-0.497648	12.010000	-2.269320
66	C	0.602248	12.713300	-1.546580
67	C	-0.461970	9.404810	1.722300
68	C	0.462703	8.655080	-1.583740

	69	C	0.673535	12.684200	0.998658
	70	C	-0.384635	11.964100	1.765620
	71	C	-0.573638	9.450130	-2.279200
	72	C	2.332970	9.857300	-0.353777
	73	C	-2.242330	10.750700	0.532664
	74	C	-2.284040	10.767500	-0.962047
	75	C	2.388760	11.361600	-0.338078
	76	C	1.691220	9.434250	-1.596140
	77	C	-1.781290	9.477730	-1.428060
	78	C	1.878940	11.824400	0.954600
	79	C	-1.635030	12.009200	0.986939
	80	C	1.761470	9.405440	0.912792
	81	C	1.807440	11.853500	-1.589220
	82	C	-1.714920	9.451310	0.940553
	83	C	-1.702440	12.036500	-1.420960
	84	C	-0.112751	7.955980	-0.306758
	85	C	0.155465	10.653200	2.155610
	86	C	0.018955	10.708600	-2.718520
	87	C	0.074575	13.173500	-0.252739

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_4$-BS	1	U	-0.048198	3.581320	-0.236481
	2	C	-1.043120	5.634200	-1.413560
	3	C	2.417370	3.615990	-0.482088
	4	C	-0.673856	3.632370	2.160840
	5	C	-0.973590	1.437880	-1.304740
	6	C	1.469400	2.893820	1.542870
	7	C	-2.119140	3.513690	-1.513460
	8	C	-0.988370	3.507230	-2.480290
	9	C	1.443850	4.410030	1.503620
	10	C	-0.640916	1.546330	1.043590
	11	C	1.102110	4.836210	-1.979500
	12	C	1.226680	5.647750	-0.718545
	13	C	-1.898550	2.293100	0.688600
	14	C	1.295740	1.536190	-0.610636
	15	C	-0.708005	5.657650	0.937724
	16	C	-1.940000	4.853920	0.622693
	17	C	1.145350	2.275430	-1.912640
	18	C	-0.043556	0.820135	-0.213758
	19	C	-1.882780	3.592170	1.363250
	20	C	1.817200	3.571300	-1.800050
	21	C	-0.135707	6.337150	-0.355982
	22	C	2.023250	2.420840	0.274726
	23	C	-0.256992	2.248440	-2.276910
	24	C	0.087000	4.844800	1.832930
	25	C	-2.082020	4.808560	-0.818553

26	C	0.127385	2.430990	1.894980
27	C	1.982270	4.834880	0.211775
28	C	-2.040160	2.258560	-0.752971
29	C	-0.299894	4.798380	-2.343030
30	U	0.060608	-3.466100	0.186266
31	C	0.668029	-5.568160	-0.973417
32	C	1.385000	-3.201900	2.269830
33	C	0.569426	-1.482430	-1.357740
34	C	-2.360800	-3.437290	0.734694
35	C	0.982179	-1.293470	0.957214
36	C	-1.567850	-4.860500	-0.957903
37	C	-1.263430	-5.484240	0.363202
38	C	2.076740	-2.077540	0.342694
39	C	-1.362120	-1.441030	-0.002254
40	C	1.088900	-5.336620	1.327380
41	C	2.161300	-4.626750	0.570639
42	C	-1.621770	-2.308980	-1.172500
43	C	-0.843127	-2.508030	2.244560
44	C	1.634800	-3.548350	-1.666390
45	C	0.253304	-3.634820	-2.232490
46	C	-0.806273	-4.006510	2.384500
47	C	-1.788110	-2.168890	1.183290
48	C	-0.396756	-2.347970	-1.998060
49	C	0.595552	-4.430550	2.390290
50	C	1.878640	-4.758710	-0.869725
51	C	0.530649	-2.023000	2.133410
52	C	-1.755430	-4.578340	1.426690
53	C	1.792430	-2.211000	-1.101090
54	C	-0.346608	-4.898240	-1.782040
55	C	0.015973	-0.709229	-0.127156
56	C	2.297220	-3.278190	1.140910
57	C	-2.207330	-3.560700	-0.705341
58	C	0.145761	-5.906430	0.352673
59	U	0.039727	10.622100	-0.375336
60	C	-1.305380	12.774900	0.007505
61	C	1.938840	10.554700	1.214700
62	C	-1.465180	8.580540	0.020035
63	C	0.870739	10.583400	-2.709350
64	C	0.801778	8.538090	0.722443
65	C	-0.956367	11.936600	-2.169070
66	C	0.290410	12.666200	-1.748160
67	C	-0.002593	9.348740	1.701950
68	C	0.134434	8.556220	-1.735200
69	C	0.959480	12.649600	0.709144
70	C	0.095379	11.908700	1.694180
71	C	-1.053260	9.376150	-2.160720
72	C	2.243800	9.776820	-0.981405

73	C	-1.999360	10.703900	0.951811
74	C	-2.390110	10.714500	-0.483636
75	C	2.301730	11.292700	-0.986338
76	C	1.303160	9.360390	-2.020870
77	C	-1.981260	9.420640	-1.048810
78	C	2.050300	11.756200	0.377689
79	C	-1.268280	11.953100	1.206550
80	C	1.957620	9.342690	0.385598
81	C	1.395460	11.773900	-2.028620
82	C	-1.365550	9.404280	1.214080
83	C	-1.884430	11.969800	-1.056580
84	C	-0.127252	7.867200	-0.349700
85	C	0.701704	10.604700	1.966950
86	C	-0.576925	10.638500	-2.729720
87	C	0.082753	13.382800	-0.367227
88	U	0.504669	17.667800	-0.311794
89	C	-0.360632	19.773000	-1.287950
90	C	0.155051	17.634700	2.146180
91	C	-0.759682	15.688100	-1.340690
92	C	2.922510	17.401500	-0.808464
93	C	-0.181325	15.641200	0.946846
94	C	1.612450	18.830500	-2.135810
95	C	1.938990	19.537600	-0.863021
96	C	-1.365900	16.511200	0.774694
97	C	1.550120	15.494900	-0.902080
98	C	0.201023	19.683800	0.992496
99	C	-1.142660	19.062300	0.805666
100	C	1.366280	16.281500	-2.142520
101	C	2.104990	16.704700	1.263570
102	C	-1.687220	17.841500	-1.352200
103	C	-0.666653	17.755900	-2.441890
104	C	2.250740	18.202900	1.281750
105	C	2.489760	16.221900	-0.060699
106	C	-0.083868	16.417600	-2.390910
107	C	1.018570	18.775300	1.829150
108	C	-1.478190	19.103400	-0.628793
109	C	0.776348	16.366100	1.768010
110	C	2.755450	18.628800	-0.025416
111	C	-1.700940	16.553400	-0.663911
112	C	0.166014	18.964900	-2.383910
113	C	0.191809	14.911700	-0.386526
114	C	-1.135920	17.761200	1.490560
115	C	2.192110	17.481000	-2.062500
116	C	0.693192	20.108000	-0.327314

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_4$-triplet	1	U	-0.048957	3.580690	-0.246049
	2	C	-1.054050	5.632100	-1.417240
	3	C	2.413570	3.610710	-0.520063
	4	C	-0.646971	3.639290	2.158240
	5	C	-0.990302	1.435820	-1.297580
	6	C	1.487830	2.895650	1.517530
	7	C	-2.134510	3.513090	-1.498950
	8	C	-1.014900	3.502040	-2.478610
	9	C	1.464200	4.411790	1.474530
	10	C	-0.630125	1.550180	1.046530
	11	C	1.083270	4.829280	-2.005360
	12	C	1.223510	5.644060	-0.747960
	13	C	-1.890640	2.297860	0.703908
	14	C	1.287050	1.532440	-0.630066
	15	C	-0.692395	5.661160	0.929933
	16	C	-1.928800	4.858370	0.631229
	17	C	1.122930	2.268410	-1.932130
	18	C	-0.048889	0.819691	-0.215467
	19	C	-1.865030	3.598620	1.374670
	20	C	1.798160	3.563500	-1.830830
	21	C	-0.133953	6.336630	-0.371715
	22	C	2.026250	2.418230	0.244373
	23	C	-0.283498	2.242530	-2.280090
	24	C	0.111857	4.849570	1.818120
	25	C	-2.087370	4.809690	-0.808208
	26	C	0.149358	2.435980	1.886480
	27	C	1.988360	4.832250	0.175469
	28	C	-2.048850	2.260010	-0.735836
	29	C	-0.322700	4.792490	-2.352690
	30	U	0.059791	-3.465210	0.195045
	31	C	0.622841	-5.572590	-0.977497
	32	C	1.454440	-3.197120	2.231710
	33	C	0.520441	-1.487760	-1.372160
	34	C	-2.341800	-3.429040	0.824935
	35	C	1.011510	-1.292150	0.926980
	36	C	-1.609660	-4.859680	-0.888668
	37	C	-1.262060	-5.479710	0.423487
	38	C	2.082950	-2.080750	0.278430
	39	C	-1.364230	-1.437610	0.047592
	40	C	1.121840	-5.334290	1.306990
	41	C	2.169530	-4.629400	0.511970
	42	C	-1.665160	-2.308860	-1.110090
	43	C	-0.771827	-2.498190	2.279320
	44	C	1.570060	-3.557250	-1.709560
	45	C	0.170039	-3.642370	-2.228350

46	C	-0.733511	-3.996250	2.423110
47	C	-1.751460	-2.160520	1.249450
48	C	-0.468832	-2.353260	-1.976450
49	C	0.666776	-4.423560	2.382960
50	C	1.838020	-4.765620	-0.917559
51	C	0.598497	-2.016750	2.120180
52	C	-1.715770	-4.569130	1.499950
53	C	1.749730	-2.218390	-1.154450
54	C	-0.417095	-4.902880	-1.753490
55	C	0.010463	-0.709392	-0.126226
56	C	2.327710	-3.279310	1.072810
57	C	-2.237370	-3.557660	-0.619018
58	C	0.145022	-5.905200	0.366693
59	U	0.044020	10.621700	-0.389401
60	C	-1.314560	12.774700	-0.057067
61	C	1.884240	10.555500	1.268280
62	C	-1.474300	8.580390	-0.047824
63	C	0.958910	10.581900	-2.692030
64	C	0.766098	8.538420	0.735953
65	C	-0.886437	11.935400	-2.218920
66	C	0.344252	12.665600	-1.753470
67	C	-0.073515	9.349480	1.685350
68	C	0.187547	8.554940	-1.744340
69	C	0.923314	12.649800	0.726531
70	C	0.024136	11.909300	1.679920
71	C	-0.983787	9.374880	-2.212990
72	C	2.268450	9.776400	-0.915148
73	C	-2.042240	10.704200	0.862591
74	C	-2.380460	10.713900	-0.586177
75	C	2.326590	11.292300	-0.918664
76	C	1.365910	9.359090	-1.987760
77	C	-1.951200	9.419800	-1.135340
78	C	2.025790	11.756500	0.435155
79	C	-1.321050	11.953400	1.143030
80	C	1.933260	9.343130	0.440897
81	C	1.458520	11.772900	-1.993250
82	C	-1.418060	9.404870	1.148460
83	C	-1.854370	11.969100	-1.141040
84	C	-0.123915	7.866650	-0.368710
85	C	0.620523	10.605600	1.975230
86	C	-0.487049	10.637000	-2.764830
87	C	0.086243	13.382700	-0.381215
88	U	0.502463	17.667900	-0.295309
89	C	-0.297690	19.774100	-1.323640
90	C	-0.006329	17.632200	2.134710
91	C	-0.692226	15.689000	-1.406350
92	C	2.947630	17.402300	-0.633989

	93	C	-0.263524	15.639900	0.913883
	94	C	1.726510	18.832500	-2.042310
	95	C	1.969430	19.538400	-0.750145
	96	C	-1.434590	16.510000	0.665907
	97	C	1.584410	15.495600	-0.818894
	98	C	0.114362	19.682600	0.988580
	99	C	-1.214220	19.061100	0.713997
	100	C	1.481460	16.283500	-2.067700
	101	C	1.997090	16.703200	1.379750
	102	C	-1.617150	17.842600	-1.475970
	103	C	-0.527906	17.758000	-2.497110
	104	C	2.141120	18.201500	1.409000
	105	C	2.467160	16.221900	0.082730
	106	C	0.050434	16.419700	-2.409590
	107	C	0.875871	18.773200	1.875680
	108	C	-1.455650	19.103700	-0.739230
	109	C	0.638490	16.364100	1.796390
	110	C	2.729850	18.628800	0.137851
	111	C	-1.675590	16.553700	-0.791355
	112	C	0.299228	18.966900	-2.383850
	113	C	0.195624	14.911700	-0.393234
	114	C	-1.251900	17.759300	1.396570
	115	C	2.300290	17.482900	-1.932830
	116	C	0.691351	20.108100	-0.296033

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_5$-BS	1	U	-0.059699	3.761220	-0.072164
	2	C	-1.444300	5.827400	-0.706168
	3	C	2.024880	3.735490	-1.412820
	4	C	0.474773	3.847100	2.345410
	5	C	-1.407250	1.634130	-0.564074
	6	C	2.088740	3.052060	0.834394
	7	C	-2.485540	3.733730	-0.267202
	8	C	-1.918510	3.692060	-1.642190
	9	C	2.075260	4.568140	0.783894
	10	C	-0.040593	1.749980	1.373560
	11	C	0.194407	4.974450	-2.170860
	12	C	0.893282	5.792790	-1.118670
	13	C	-1.308600	2.524900	1.615700
	14	C	0.930697	1.683590	-0.979684
	15	C	-0.076651	5.864170	1.234950
	16	C	-1.330900	5.086090	1.529410
	17	C	0.217678	2.414640	-2.083850
	18	C	-0.093999	1.003140	-0.004774
	19	C	-0.965011	3.829060	2.185770

20	C	0.890225	3.694530	-2.312830
21	C	-0.143715	6.519120	-0.190466
22	C	1.996800	2.556420	-0.538293
23	C	-1.196950	2.418190	-1.770360
24	C	1.024490	5.038570	1.685550
25	C	-2.113850	5.032700	0.311154
26	C	1.045860	2.624130	1.766190
27	C	1.974710	4.969610	-0.618829
28	C	-2.091140	2.483580	0.397112
29	C	-1.220010	4.967010	-1.856820
30	U	0.063190	-3.280110	0.158381
31	C	-0.033209	-5.415090	-1.258130
32	C	2.243040	-3.176770	1.332100
33	C	-0.175198	-1.227930	-1.360060
34	C	-1.794590	-3.304100	1.797210
35	C	1.317040	-1.169410	0.484514
36	C	-1.941590	-4.637150	-0.116180
37	C	-1.070720	-5.361450	0.875688
38	C	1.946370	-1.953260	-0.636229
39	C	-1.210810	-1.249510	0.776654
40	C	1.457350	-5.281160	0.585424
41	C	2.033660	-4.513030	-0.573308
42	C	-2.028720	-2.077250	-0.177771
43	C	0.300343	-2.457370	2.440200
44	C	0.539273	-3.322100	-2.228440
45	C	-0.938344	-3.368010	-2.058390
46	C	0.352522	-3.973090	2.477000
47	C	-1.023070	-2.064880	1.958000
48	C	-1.340520	-2.091190	-1.452870
49	C	1.535590	-4.400230	1.731310
50	C	1.075690	-4.565790	-1.659040
51	C	1.452550	-1.986790	1.672390
52	C	-0.940134	-4.478310	2.016260
53	C	0.988846	-2.018720	-1.721460
54	C	-1.253790	-4.638260	-1.391360
55	C	-0.038082	-0.525261	0.026360
56	C	2.482790	-3.203710	-0.096227
57	C	-2.350490	-3.355130	0.460455
58	C	0.150452	-6.038660	0.160343
59	U	0.081910	10.811200	-0.451183
60	C	-0.959452	12.920600	0.323539
61	C	2.458140	10.696000	0.258883
62	C	-1.173650	8.829160	0.585190
63	C	-0.053944	10.625100	-2.923450
64	C	1.171940	8.729960	0.352117
65	C	-1.525860	12.056700	-1.781870
66	C	-0.201145	12.734500	-1.893230

67	C	0.846600	9.573850	1.523800
68	C	-0.399476	8.686790	-1.639750
69	C	1.376470	12.779200	0.105134
70	C	0.975076	12.127800	1.386130
71	C	-1.633360	9.503280	-1.618250
72	C	1.853920	9.845330	-1.828680
73	C	-1.270150	10.957200	1.565720
74	C	-2.196530	10.930600	0.392042
75	C	1.931660	11.345800	-1.923460
76	C	0.590375	9.412670	-2.420640
77	C	-2.092220	9.607300	-0.217463
78	C	2.302680	11.868300	-0.606581
79	C	-0.491913	12.201900	1.505250
80	C	2.145450	9.456300	-0.450758
81	C	0.725910	11.823900	-2.603890
82	C	-0.624306	9.649410	1.642390
83	C	-1.984510	12.159600	-0.385094
84	C	-0.108763	8.051040	-0.238674
85	C	1.620340	10.807500	1.441180
86	C	-1.400650	10.721900	-2.385610
87	C	0.156234	13.255200	-0.564596
88	U	0.178907	-10.324000	0.294864
89	C	1.399750	-12.429600	-0.520510
90	C	0.202504	-10.274300	2.771590
91	C	1.366490	-8.234890	-0.603238
92	C	-2.153910	-10.360400	-0.541918
93	C	0.471597	-8.236540	1.595520
94	C	-0.532234	-11.649300	-1.623290
95	C	-0.970891	-12.404800	-0.397782
96	C	1.766860	-9.004220	1.588170
97	C	-1.004610	-8.293970	-0.478974
98	C	0.503928	-12.352200	1.677520
99	C	1.786910	-11.566300	1.639330
100	C	-0.553145	-9.088520	-1.673510
101	C	-1.715420	-9.554340	1.621190
102	C	2.498470	-10.320900	-0.442187
103	C	1.636440	-10.351600	-1.654520
104	C	-1.703140	-11.071000	1.651990
105	C	-1.938040	-9.135290	0.237982
106	C	0.895688	-9.082720	-1.686560
107	C	-0.473312	-11.497100	2.318520
108	C	2.275390	-11.584100	0.275129
109	C	-0.492657	-9.081800	2.269680
110	C	-1.917860	-11.549400	0.286729
111	C	2.254980	-9.034060	0.224388
112	C	0.916459	-11.632400	-1.636420
113	C	0.208370	-7.566780	0.201736

	114	C	1.569330	-10.273300	2.291380
	115	C	-1.251020	-10.375300	-1.674920
	116	C	0.253296	-13.084700	0.311501
	117	U	0.019701	-17.384000	0.340211
	118	C	1.230670	-19.448500	0.976399
	119	C	-2.140800	-17.227700	1.553690
	120	C	1.451590	-15.349400	0.963534
	121	C	-0.399073	-17.334300	-2.106740
	122	C	-0.888190	-15.260500	1.252930
	123	C	1.305680	-18.702300	-1.245700
	124	C	-0.003072	-19.383900	-1.023070
	125	C	-0.301238	-16.039300	2.366550
	126	C	0.201031	-15.328700	-1.037910
	127	C	-1.096920	-19.317200	1.275580
	128	C	-0.428394	-18.596700	2.398340
	129	C	1.418020	-16.143800	-1.247610
	130	C	-2.024830	-16.493600	-0.658611
	131	C	1.787420	-17.420200	2.010930
	132	C	2.429650	-17.459000	0.660939
	133	C	-2.104870	-17.997000	-0.652965
	134	C	-0.929282	-16.095400	-1.539180
	135	C	2.177650	-16.171100	0.019647
	136	C	-2.168250	-18.445900	0.739618
	137	C	1.029260	-18.665700	2.192190
	138	C	-2.007390	-16.029100	0.726677
	139	C	-1.074990	-18.512900	-1.557750
	140	C	1.160040	-16.109700	2.158970
	141	C	2.064100	-18.728600	0.017665
	142	C	0.221547	-14.616700	0.356751
	143	C	-1.060140	-17.274900	2.524380
	144	C	1.034500	-17.402600	-1.877430
	145	C	-0.050628	-19.830400	0.377914

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_5$-triplet	1	U	-0.059699	3.761220	-0.072164
	2	C	-1.444300	5.827400	-0.706168
	3	C	2.024880	3.735490	-1.412820
	4	C	0.474773	3.847100	2.345410
	5	C	-1.407250	1.634130	-0.564074
	6	C	2.088740	3.052060	0.834394
	7	C	-2.485540	3.733730	-0.267202
	8	C	-1.918510	3.692060	-1.642190
	9	C	2.075260	4.568140	0.783894
	10	C	-0.040593	1.749980	1.373560

11	C	0.194407	4.974450	-2.170860
12	C	0.893282	5.792790	-1.118670
13	C	-1.308600	2.524900	1.615700
14	C	0.930697	1.683590	-0.979684
15	C	-0.076651	5.864170	1.234950
16	C	-1.330900	5.086090	1.529410
17	C	0.217678	2.414640	-2.083850
18	C	-0.093999	1.003140	-0.004774
19	C	-0.965011	3.829060	2.185770
20	C	0.890225	3.694530	-2.312830
21	C	-0.143715	6.519120	-0.190466
22	C	1.996800	2.556420	-0.538293
23	C	-1.196950	2.418190	-1.770360
24	C	1.024490	5.038570	1.685550
25	C	-2.113850	5.032700	0.311154
26	C	1.045860	2.624130	1.766190
27	C	1.974710	4.969610	-0.618829
28	C	-2.091140	2.483580	0.397112
29	C	-1.220010	4.967010	-1.856820
30	U	0.063190	-3.280110	0.158381
31	C	-0.033209	-5.415090	-1.258130
32	C	2.243040	-3.176770	1.332100
33	C	-0.175198	-1.227930	-1.360060
34	C	-1.794590	-3.304100	1.797210
35	C	1.317040	-1.169410	0.484514
36	C	-1.941590	-4.637150	-0.116180
37	C	-1.070720	-5.361450	0.875688
38	C	1.946370	-1.953260	-0.636229
39	C	-1.210810	-1.249510	0.776654
40	C	1.457350	-5.281160	0.585424
41	C	2.033660	-4.513030	-0.573308
42	C	-2.028720	-2.077250	-0.177771
43	C	0.300343	-2.457370	2.440200
44	C	0.539273	-3.322100	-2.228440
45	C	-0.938344	-3.368010	-2.058390
46	C	0.352522	-3.973090	2.477000
47	C	-1.023070	-2.064880	1.958000
48	C	-1.340520	-2.091190	-1.452870
49	C	1.535590	-4.400230	1.731310
50	C	1.075690	-4.565790	-1.659040
51	C	1.452550	-1.986790	1.672390
52	C	-0.940134	-4.478310	2.016260
53	C	0.988846	-2.018720	-1.721460
54	C	-1.253790	-4.638260	-1.391360
55	C	-0.038082	-0.525261	0.026360
56	C	2.482790	-3.203710	-0.096227
57	C	-2.350490	-3.355130	0.460455

58	C	0.150452	-6.038660	0.160343
59	U	0.081910	10.811200	-0.451183
60	C	-0.959452	12.920600	0.323539
61	C	2.458140	10.696000	0.258883
62	C	-1.173650	8.829160	0.585190
63	C	-0.053944	10.625100	-2.923450
64	C	1.171940	8.729960	0.352117
65	C	-1.525860	12.056700	-1.781870
66	C	-0.201145	12.734500	-1.893230
67	C	0.846600	9.573850	1.523800
68	C	-0.399476	8.686790	-1.639750
69	C	1.376470	12.779200	0.105134
70	C	0.975076	12.127800	1.386130
71	C	-1.633360	9.503280	-1.618250
72	C	1.853920	9.845330	-1.828680
73	C	-1.270150	10.957200	1.565720
74	C	-2.196530	10.930600	0.392042
75	C	1.931660	11.345800	-1.923460
76	C	0.590375	9.412670	-2.420640
77	C	-2.092220	9.607300	-0.217463
78	C	2.302680	11.868300	-0.606581
79	C	-0.491913	12.201900	1.505250
80	C	2.145450	9.456300	-0.450758
81	C	0.725910	11.823900	-2.603890
82	C	-0.624306	9.649410	1.642390
83	C	-1.984510	12.159600	-0.385094
84	C	-0.108763	8.051040	-0.238674
85	C	1.620340	10.807500	1.441180
86	C	-1.400650	10.721900	-2.385610
87	C	0.156234	13.255200	-0.564596
88	U	0.178907	-10.324000	0.294864
89	C	1.399750	-12.429600	-0.520510
90	C	0.202504	-10.274300	2.771590
91	C	1.366490	-8.234890	-0.603238
92	C	-2.153910	-10.360400	-0.541918
93	C	0.471597	-8.236540	1.595520
94	C	-0.532234	-11.649300	-1.623290
95	C	-0.970891	-12.404800	-0.397782
96	C	1.766860	-9.004220	1.588170
97	C	-1.004610	-8.293970	-0.478974
98	C	0.503928	-12.352200	1.677520
99	C	1.786910	-11.566300	1.639330
100	C	-0.553145	-9.088520	-1.673510
101	C	-1.715420	-9.554340	1.621190
102	C	2.498470	-10.320900	-0.442187
103	C	1.636440	-10.351600	-1.654520
104	C	-1.703140	-11.071000	1.651990

	105	C	-1.938040	-9.135290	0.237982
	106	C	0.895688	-9.082720	-1.686560
	107	C	-0.473312	-11.497100	2.318520
	108	C	2.275390	-11.584100	0.275129
	109	C	-0.492657	-9.081800	2.269680
	110	C	-1.917860	-11.549400	0.286729
	111	C	2.254980	-9.034060	0.224388
	112	C	0.916459	-11.632400	-1.636420
	113	C	0.208370	-7.566780	0.201736
	114	C	1.569330	-10.273300	2.291380
	115	C	-1.251020	-10.375300	-1.674920
	116	C	0.253296	-13.084700	0.311501
	117	U	0.019701	-17.384000	0.340211
	118	C	1.230670	-19.448500	0.976399
	119	C	-2.140800	-17.227700	1.553690
	120	C	1.451590	-15.349400	0.963534
	121	C	-0.399073	-17.334300	-2.106740
	122	C	-0.888190	-15.260500	1.252930
	123	C	1.305680	-18.702300	-1.245700
	124	C	-0.003072	-19.383900	-1.023070
	125	C	-0.301238	-16.039300	2.366550
	126	C	0.201031	-15.328700	-1.037910
	127	C	-1.096920	-19.317200	1.275580
	128	C	-0.428394	-18.596700	2.398340
	129	C	1.418020	-16.143800	-1.247610
	130	C	-2.024830	-16.493600	-0.658611
	131	C	1.787420	-17.420200	2.010930
	132	C	2.429650	-17.459000	0.660939
	133	C	-2.104870	-17.997000	-0.652965
	134	C	-0.929282	-16.095400	-1.539180
	135	C	2.177650	-16.171100	0.019647
	136	C	-2.168250	-18.445900	0.739618
	137	C	1.029260	-18.665700	2.192190
	138	C	-2.007390	-16.029100	0.726677
	139	C	-1.074990	-18.512900	-1.557750
	140	C	1.160040	-16.109700	2.158970
	141	C	2.064100	-18.728600	0.017665
	142	C	0.221547	-14.616700	0.356751
	143	C	-1.060140	-17.274900	2.524380
	144	C	1.034500	-17.402600	-1.877430
	145	C	-0.050628	-19.830400	0.377914

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_6$-BS	1	U	-0.290230	3.690367	-0.376941

2	C	-1.750461	5.789497	-0.522706
3	C	1.352928	3.719846	-2.208077
4	C	0.849508	3.647718	1.803657
5	C	-1.760644	1.605253	-0.598236
6	C	1.987993	2.927821	-0.104604
7	C	-2.673530	3.688277	0.068404
8	C	-2.489589	3.714168	-1.396642
9	C	1.991595	4.431394	-0.077023
10	C	0.059567	1.620938	0.902500
11	C	-0.574444	5.002084	-2.394641
12	C	0.383918	5.755503	-1.527663
13	C	-1.076151	2.383890	1.506962
14	C	0.374532	1.665237	-1.602134
15	C	0.069985	5.710031	0.977196
16	C	-1.069682	4.931496	1.553225
17	C	-0.580403	2.454034	-2.440867
18	C	-0.365827	0.937118	-0.435617
19	C	-0.574325	3.647390	2.023124
20	C	0.027572	3.733161	-2.772447
21	C	-0.352476	6.444182	-0.334735
22	C	1.529030	2.502989	-1.419117
23	C	-1.856759	2.450685	-1.767131
24	C	1.226217	4.861835	1.084057
25	C	-2.140107	4.946245	0.585262
26	C	1.220381	2.458843	1.040002
27	C	1.534744	4.906258	-1.375053
28	C	-2.146420	2.409922	0.539194
29	C	-1.850647	4.987043	-1.721095
30	U	-0.128596	-3.337610	-0.310296
31	C	-0.578460	-5.494731	-1.614569
32	C	2.272757	-3.190201	0.205775
33	C	-0.809176	-1.318626	-1.730845
34	C	-1.456084	-3.353527	1.761169
35	C	1.120081	-1.221159	-0.376547
36	C	-2.099439	-4.714766	-0.007038
37	C	-0.981941	-5.405710	0.708139
38	C	1.429655	-2.011040	-1.608662
39	C	-1.208129	-1.322994	0.594985
40	C	1.346450	-5.303911	-0.262592
41	C	1.570433	-4.554492	-1.537583
42	C	-2.240182	-2.171347	-0.077593
43	C	0.709519	-2.479344	1.788982
44	C	-0.331523	-3.416042	-2.725051
45	C	-1.693505	-3.475365	-2.156992
46	C	0.792810	-3.980387	1.830622
47	C	-0.694523	-2.109310	1.683969
48	C	-1.929674	-2.198932	-1.486818

49	C	1.724525	-4.408312	0.797216
50	C	0.354504	-4.637331	-2.310629
51	C	1.591287	-2.009180	0.730404
52	C	-0.561361	-4.508447	1.750620
53	C	0.214393	-2.105611	-2.381161
54	C	-1.789530	-4.730736	-1.416434
55	C	-0.307828	-0.592052	-0.450943
56	C	2.106779	-3.239362	-1.224355
57	C	-2.350807	-3.434404	0.635111
58	C	-0.002640	-6.089585	-0.298244
59	U	-0.046243	10.716619	-0.352867
60	C	-0.776408	12.866218	0.830241
61	C	2.406558	10.541399	-0.269949
62	C	-1.074933	8.693705	0.833142
63	C	-0.828292	10.770985	-2.685006
64	C	1.124998	8.582981	-0.011410
65	C	-1.868271	12.123891	-1.109729
66	C	-0.602501	12.806216	-1.522468
67	C	1.133556	9.356102	1.269015
68	C	-0.894407	8.725634	-1.519681
69	C	1.417135	12.662559	-0.014011
70	C	1.315390	11.897589	1.267516
71	C	-2.049925	9.581965	-1.107977
72	C	1.268933	9.867456	-2.195446
73	C	-0.831210	10.774279	1.940501
74	C	-2.012553	10.858149	1.058385
75	C	1.376232	11.367408	-2.196359
76	C	-0.122331	9.515679	-2.440386
77	C	-2.092258	9.591735	0.334611
78	C	2.032238	11.772494	-0.961709
79	C	-0.051169	11.989667	1.721801
80	C	1.860764	9.375006	-0.959955
81	C	0.049404	11.913329	-2.442140
82	C	-0.232269	9.459878	1.723362
83	C	-1.911251	12.121781	0.332765
84	C	-0.284489	7.972520	-0.295164
85	C	1.897576	10.578628	1.077198
86	C	-1.969719	10.853296	-1.810048
87	C	0.108502	13.466381	-0.298742
88	U	0.179569	-10.348278	0.122383
89	C	1.173559	-12.501501	-0.841602
90	C	0.919645	-10.088715	2.454610
91	C	0.991478	-8.341646	-1.245980
92	C	-2.275319	-10.467679	0.005093
93	C	0.772169	-8.170470	1.096845
94	C	-1.007141	-11.828234	-1.385687
95	C	-1.044043	-12.474347	-0.036965

96	C	2.025854	-8.922053	0.778638
97	C	-1.222766	-8.407118	-0.432312
98	C	0.950813	-12.237773	1.493050
99	C	2.136984	-11.455866	1.025397
100	C	-1.118436	-9.294423	-1.631785
101	C	-1.258305	-9.485728	1.864270
102	C	2.175022	-10.394589	-1.253992
103	C	1.008403	-10.532536	-2.148560
104	C	-1.192470	-10.981026	2.009891
105	C	-1.879917	-9.185389	0.582665
106	C	0.258541	-9.281662	-2.064080
107	C	0.183608	-11.343082	2.317059
108	C	2.206089	-11.586545	-0.410156
109	C	0.078616	-8.953096	2.084252
110	C	-1.774681	-11.575354	0.815494
111	C	2.095569	-9.064403	-0.655728
112	C	0.369076	-11.803878	-1.819066
113	C	0.101643	-7.613201	-0.199188
114	C	2.078955	-10.121116	1.600057
115	C	-1.740492	-10.573685	-1.328483
116	C	0.343004	-13.089797	0.333885
117	U	0.247425	-17.363878	0.845460
118	C	1.650097	-19.332856	1.277690
119	C	-1.426517	-17.068597	2.629081
120	C	1.745068	-15.278481	0.795085
121	C	-0.886255	-17.553720	-1.333697
122	C	-0.387461	-15.160057	1.768274
123	C	1.025589	-18.824876	-0.907241
124	C	-0.122869	-19.469876	-0.234929
125	C	0.524221	-15.814988	2.714909
126	C	-0.050437	-15.463188	-0.706584
127	C	-0.462596	-19.165027	2.256975
128	C	0.487938	-18.342439	3.035760
129	C	1.057320	-16.293428	-1.195788
130	C	-2.011261	-16.574067	0.440880
131	C	2.432976	-17.223453	1.880356
132	C	2.631799	-17.401648	0.421528
133	C	-2.039815	-18.054380	0.618257
134	C	-1.250885	-16.268694	-0.761256
135	C	2.169974	-16.189805	-0.231176
136	C	-1.664732	-18.356177	1.993160
137	C	1.806775	-18.434517	2.406077
138	C	-1.585517	-15.968141	1.693178
139	C	-1.325197	-18.661020	-0.496925
140	C	1.854616	-15.907198	2.082087
141	C	2.127941	-18.722445	0.051241
142	C	0.372392	-14.607259	0.524976

	143	C	-0.106581	-17.016781	3.217036
	144	C	0.543123	-17.599823	-1.547435
	145	C	0.267857	-19.766910	1.142452
	146	U	0.695609	17.730928	-0.382270
	147	C	-0.470123	19.880940	-0.604960
	148	C	1.832991	17.569475	1.797182
	149	C	-1.031116	15.836311	-0.531632
	150	C	2.333312	17.427090	-2.197808
	151	C	0.766454	15.662342	0.968579
	152	C	0.579439	18.946130	-2.461435
	153	C	1.614186	19.571855	-1.610268
	154	C	-0.241366	16.560162	1.546482
	155	C	1.078341	15.572898	-1.526510
	156	C	1.299494	19.661269	0.901893
	157	C	0.081431	19.087503	1.513572
	158	C	0.252300	16.420028	-2.396168
	159	C	2.847043	16.651089	-0.074492
	160	C	-1.670790	17.998525	0.059300
	161	C	-1.486497	17.946407	-1.411345
	162	C	3.045806	18.128692	-0.102238
	163	C	2.360608	16.227067	-1.378419
	164	C	-1.061834	16.599558	-1.748275
	165	C	2.400018	18.697741	1.073152
	166	C	-1.020690	19.208895	0.557078
	167	C	2.050926	16.315389	1.095973
	168	C	2.714349	18.608270	-1.437211
	169	C	-1.354008	16.682227	0.583755
	170	C	-0.723215	19.124553	-1.816869
	171	C	0.254084	14.988643	-0.339795
	172	C	0.417342	17.757084	2.024145
	173	C	1.019032	17.586155	-2.779197
	174	C	0.952147	20.138079	-0.435964

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_6$-triplet	1	U	-0.290294	3.690376	-0.376694
	2	C	-1.750611	5.789507	-0.521899
	3	C	1.352142	3.719864	-2.208463
	4	C	0.850263	3.647730	1.803465
	5	C	-1.760806	1.605251	-0.597426
	6	C	1.988022	2.927844	-0.105235
	7	C	-2.673441	3.688277	0.069564
	8	C	-2.490059	3.714168	-1.395553
	9	C	1.991626	4.431413	-0.077654
	10	C	0.059980	1.620949	0.902603

11	C	-0.575309	5.002094	-2.394286
12	C	0.383380	5.755516	-1.527674
13	C	-1.075509	2.383896	1.507508
14	C	0.373987	1.665250	-1.602144
15	C	0.070412	5.710041	0.977299
16	C	-1.069029	4.931502	1.553771
17	C	-0.581272	2.454041	-2.440511
18	C	-0.365926	0.937119	-0.435342
19	C	-0.573489	3.647397	2.023476
20	C	0.026565	3.733173	-2.772324
21	C	-0.352557	6.444198	-0.334464
22	C	1.528556	2.503004	-1.419573
23	C	-1.857367	2.450686	-1.766280
24	C	1.226693	4.861853	1.083724
25	C	-2.139823	4.946247	0.586216
26	C	1.220850	2.458854	1.039669
27	C	1.534274	4.906282	-1.375509
28	C	-2.146146	2.409925	0.540148
29	C	-1.851250	4.987047	-1.720246
30	U	-0.128598	-3.337607	-0.310154
31	C	-0.578978	-5.494715	-1.614290
32	C	2.272959	-3.190184	0.204919
33	C	-0.809783	-1.318606	-1.730415
34	C	-1.455245	-3.353569	1.761836
35	C	1.120016	-1.221148	-0.376904
36	C	-2.099312	-4.714787	-0.006130
37	C	-0.981521	-5.405733	0.708578
38	C	1.429102	-2.011004	-1.609157
39	C	-1.207787	-1.323013	0.595585
40	C	1.346483	-5.303901	-0.263103
41	C	1.569935	-4.554454	-1.538173
42	C	-2.240105	-2.171364	-0.076585
43	C	0.710362	-2.479372	1.788779
44	C	-0.332519	-3.416007	-2.724841
45	C	-1.694269	-3.475349	-2.156225
46	C	0.793684	-3.980413	1.830360
47	C	-0.693728	-2.109341	1.684350
48	C	-1.930171	-2.198925	-1.485937
49	C	1.724985	-4.408314	0.796567
50	C	0.353689	-4.637293	-2.310719
51	C	1.591695	-2.009175	0.729848
52	C	-0.560520	-4.508487	1.750904
53	C	0.213524	-2.105579	-2.381156
54	C	-1.789974	-4.730733	-1.415650
55	C	-0.307915	-0.592042	-0.450709
56	C	2.106394	-3.239323	-1.225147
57	C	-2.350428	-3.434436	0.636140

58	C	-0.002622	-6.089588	-0.298219
59	U	-0.046279	10.716626	-0.352793
60	C	-0.776100	12.866264	0.830461
61	C	2.406538	10.541377	-0.270510
62	C	-1.074679	8.693756	0.833564
63	C	-0.828963	10.770943	-2.684709
64	C	1.125010	8.582989	-0.011573
65	C	-1.868504	12.123902	-1.109188
66	C	-0.602843	12.806206	-1.522291
67	C	1.133930	9.356145	1.268832
68	C	-0.894797	8.725618	-1.519322
69	C	1.417211	12.662558	-0.014359
70	C	1.315799	11.897622	1.267212
71	C	-2.050186	9.581975	-1.107319
72	C	1.268384	9.867402	-2.195688
73	C	-0.830636	10.774362	1.940799
74	C	-2.012216	10.858220	1.058996
75	C	1.375702	11.367353	-2.196666
76	C	-0.122954	9.515634	-2.440247
77	C	-2.092127	9.591784	0.335280
78	C	2.032051	11.772462	-0.962201
79	C	-0.050638	11.989730	1.721857
80	C	1.860544	9.374970	-0.960339
81	C	0.048811	11.913287	-2.442109
82	C	-0.231771	9.459952	1.723538
83	C	-1.911092	12.121830	0.333317
84	C	-0.284545	7.972531	-0.294927
85	C	1.897914	10.578650	1.076774
86	C	-1.970155	10.853289	-1.809443
87	C	0.108508	13.466389	-0.298762
88	U	0.179615	-10.348280	0.122344
89	C	1.173430	-12.501507	-0.841822
90	C	0.920082	-10.088743	2.454443
91	C	0.991341	-8.341651	-1.246144
92	C	-2.275284	-10.467650	0.005429
93	C	0.772420	-8.170487	1.096714
94	C	-1.007344	-11.828209	-1.385566
95	C	-1.044043	-12.474337	-0.036847
96	C	2.026042	-8.922091	0.778299
97	C	-1.222776	-8.407099	-0.432131
98	C	0.951067	-12.237797	1.492866
99	C	2.137173	-11.455902	1.025027
100	C	-1.118646	-9.294396	-1.631624
101	C	-1.257959	-9.485726	1.864452
102	C	2.174858	-10.394610	-1.254363
103	C	1.008094	-10.532533	-2.148747
104	C	-1.192120	-10.981027	2.010052

105	C	-1.879775	-9.185367	0.582947
106	C	0.258263	-9.281651	-2.064134
107	C	0.184006	-11.343102	2.317003
108	C	2.206043	-11.586570	-0.410538
109	C	0.079011	-8.953108	2.084228
110	C	-1.774531	-11.575341	0.815740
111	C	2.095521	-9.064430	-0.656079
112	C	0.368806	-11.803869	-1.819160
113	C	0.101691	-7.613200	-0.199210
114	C	2.079255	-10.121157	1.599701
115	C	-1.740667	-10.573651	-1.328236
116	C	0.343059	-13.089805	0.333783
117	U	0.247410	-17.363873	0.845307
118	C	1.650073	-19.332918	1.277333
119	C	-1.426297	-17.068579	2.629141
120	C	1.745113	-15.278544	0.794782
121	C	-0.886538	-17.553654	-1.333713
122	C	-0.387280	-15.160047	1.768260
123	C	1.025315	-18.824886	-0.907508
124	C	-0.123085	-19.469858	-0.235070
125	C	0.524498	-15.815041	2.714758
126	C	-0.050565	-15.463156	-0.706681
127	C	-0.462495	-19.165040	2.256882
128	C	0.488164	-18.342498	3.035559
129	C	1.057101	-16.293438	-1.196028
130	C	-2.011282	-16.573974	0.441020
131	C	2.433098	-17.223552	1.879942
132	C	2.631737	-17.401732	0.421082
133	C	-2.039876	-18.054293	0.618374
134	C	-1.251054	-16.268613	-0.761218
135	C	2.169864	-16.189872	-0.231544
136	C	-1.664638	-18.356134	1.993227
137	C	1.806920	-18.434609	2.405721
138	C	-1.585375	-15.968086	1.693285
139	C	-1.325420	-18.660947	-0.496908
140	C	1.854800	-15.907289	2.081764
141	C	2.127789	-18.722510	0.050835
142	C	0.372440	-14.607268	0.524855
143	C	-0.106286	-17.016825	3.216940
144	C	0.542813	-17.599810	-1.547630
145	C	0.267801	-19.766921	1.142257
146	U	0.695709	17.730905	-0.382541
147	C	-0.470020	19.880952	-0.605065
148	C	1.833511	17.569500	1.796687
149	C	-1.031093	15.836346	-0.531501
150	C	2.333035	17.426988	-2.198398
151	C	0.766754	15.662366	0.968361

	152	C	0.579149	18.946069	-2.461716
	153	C	1.614084	19.571792	-1.610777
	154	C	-0.240924	16.560239	1.546434
	155	C	1.078151	15.572833	-1.526814
	156	C	1.299891	19.661288	0.901446
	157	C	0.081934	19.087569	1.513377
	158	C	0.251957	16.419973	-2.396319
	159	C	2.847159	16.651024	-0.075163
	160	C	-1.670603	17.998589	0.059491
	161	C	-1.486603	17.946421	-1.411192
	162	C	3.045963	18.128622	-0.102989
	163	C	2.360466	16.226975	-1.378989
	164	C	-1.062032	16.599559	-1.748162
	165	C	2.400425	18.697726	1.072514
	166	C	-1.020374	19.208962	0.557104
	167	C	2.051278	16.315376	1.095483
	168	C	2.714259	18.608177	-1.437913
	169	C	-1.353746	16.682307	0.583924
	170	C	-0.723372	19.124543	-1.816904
	171	C	0.254108	14.988645	-0.339896
	172	C	0.417912	17.757159	2.023930
	173	C	1.018644	17.586074	-2.779533
	174	C	0.952290	20.138058	-0.436358

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_7$-BS	1	U	-0.005209	-0.560087	-0.010630
	2	C	-2.065426	-2.077215	0.088953
	3	C	-0.121169	0.828847	-2.039255
	4	C	0.055176	0.856246	2.000780
	5	C	2.113404	-1.996136	-0.093028
	6	C	0.700954	1.752321	-0.057225
	7	C	0.072301	-2.863039	0.740610
	8	C	0.008209	-2.873614	-0.734395
	9	C	-0.802181	1.723076	0.008476
	10	C	2.083162	0.004953	1.159063
	11	C	-1.353492	-1.136970	-1.939855
	12	C	-2.113079	-0.092045	-1.186116
	13	C	1.364203	-1.060355	1.924483
	14	C	1.972284	-0.011878	-1.365282
	15	C	-2.004039	-0.073776	1.337932
	16	C	-1.181039	-1.109607	2.035766
	17	C	1.191443	-1.087468	-2.050994
	18	C	2.745688	-0.575255	-0.131403
	19	C	0.099256	-0.525901	2.404089

20	C	-0.110750	-0.558797	-2.425725
21	C	-2.753597	-0.682589	0.109885
22	C	1.107471	1.135576	-1.311433
23	C	1.244960	-2.264385	-1.217130
24	C	-1.184565	1.105992	1.269919
25	C	-1.187691	-2.297411	1.216209
26	C	1.215894	1.152530	1.164799
27	C	-1.292834	1.089369	-1.206494
28	C	1.346202	-2.248466	1.105786
29	C	-1.288632	-2.313698	-1.106874
30	U	7.017254	-0.260213	-0.180984
31	C	9.138416	-0.862370	-1.483359
32	C	6.844619	2.187586	0.000566
33	C	4.965344	-1.158776	-1.422758
34	C	7.123151	-1.284517	2.054226
35	C	4.877261	0.940987	-0.347847
36	C	8.436818	-2.151836	0.347214
37	C	9.131613	-0.936414	0.875156
38	C	5.622756	1.083814	-1.637014
39	C	5.051714	-1.228013	0.936164
40	C	8.958372	1.233038	-0.406405
41	C	8.164553	1.265168	-1.673377
42	C	5.895665	-2.332596	0.384376
43	C	6.211913	0.852504	1.809513
44	C	7.021156	-0.798519	-2.544143
45	C	7.121946	-2.066431	-1.794095
46	C	7.712480	0.959890	1.787422
47	C	5.864255	-0.556941	1.914250
48	C	5.872337	-2.222176	-1.054247
49	C	8.090049	1.742636	0.620274
50	C	8.243352	-0.045866	-2.271565
51	C	5.693096	1.571448	0.655373
52	C	8.261121	-0.385241	1.879580
53	C	5.713025	-0.226183	-2.235681
54	C	8.402300	-2.043004	-1.091234
55	C	4.272802	-0.491891	-0.199806
56	C	6.850994	1.824165	-1.393334
57	C	7.182601	-2.326766	1.062066
58	C	9.764719	-0.100158	-0.279747
59	U	-7.033680	-0.536962	0.124984
60	C	-9.143098	-1.215016	1.410540
61	C	-6.955780	1.915369	-0.064095
62	C	-4.960195	-1.350082	1.390373
63	C	-7.077554	-1.572019	-2.107165
64	C	-4.944759	0.748061	0.307498
65	C	-8.373111	-2.483961	-0.408861
66	C	-9.109261	-1.299781	-0.949107

67	C	-5.706997	0.866058	1.588994
68	C	-5.021712	-1.430519	-0.968878
69	C	-9.033795	0.879421	0.326166
70	C	-8.253875	0.948051	1.600974
71	C	-5.826596	-2.565692	-0.421076
72	C	-6.253706	0.600010	-1.861816
73	C	-7.039310	-1.066177	2.490486
74	C	-7.084002	-2.339519	1.744744
75	C	-7.757681	0.647925	-1.855181
76	C	-5.849692	-0.795065	-1.957957
77	C	-5.821728	-2.449434	1.017319
78	C	-8.176751	1.419598	-0.694344
79	C	-8.286954	-0.362519	2.204103
80	C	-5.774998	1.342578	-0.705415
81	C	-8.251551	-0.718129	-1.946316
82	C	-5.751521	-0.444229	2.192082
83	C	-8.357479	-2.367766	1.029342
84	C	-4.283110	-0.660355	0.170709
85	C	-6.960988	1.556449	1.331042
86	C	-7.105742	-2.612524	-1.111539
87	C	-9.785758	-0.484007	0.197122
88	U	14.034277	0.194298	-0.100922
89	C	16.112184	1.110290	-1.284980
90	C	13.880912	1.183990	2.146807
91	C	11.941456	0.817922	-1.439994
92	C	14.201230	-2.255910	0.046880
93	C	11.897117	0.857163	0.920135
94	C	15.459588	-1.128587	-1.546738
95	C	16.175014	-1.004827	-0.239304
96	C	12.604300	2.079135	0.424971
97	C	12.097937	-1.292312	-0.390815
98	C	15.976024	1.142988	1.072895
99	C	15.144468	2.256797	0.520196
100	C	12.919020	-1.307122	-1.641469
101	C	13.295122	-1.054899	1.833203
102	C	13.964875	2.024357	-1.688322
103	C	14.081573	0.767812	-2.455283
104	C	14.794942	-0.949461	1.889526
105	C	12.942654	-1.819547	0.646449
106	C	12.853267	0.012647	-2.221047
107	C	15.141992	0.457428	2.023621
108	C	15.198006	2.168301	-0.919075
109	C	12.746305	0.289534	1.933025
110	C	15.338023	-1.650806	0.736077
111	C	12.669834	1.991417	-1.013658
112	C	15.382297	0.190160	-2.127139
113	C	11.289256	0.036960	-0.262507

114	C	13.843372	2.242115	1.169858
115	C	14.225899	-1.871276	-1.340882
116	C	16.778316	0.423431	-0.057319
117	U	21.077421	0.484642	0.171025
118	C	23.020334	1.967445	0.393990
119	C	20.961794	-1.102013	2.052613
120	C	18.942471	1.911694	0.189389
121	C	21.158651	-0.756981	-1.955522
122	C	18.962893	-0.170643	1.275459
123	C	22.387575	1.214499	-1.716210
124	C	23.117547	0.123009	-1.033573
125	C	19.649322	0.810241	2.126804
126	C	19.086965	0.043790	-1.229458
127	C	22.993913	-0.094406	1.488679
128	C	22.192239	0.870868	2.273515
129	C	19.842771	1.150534	-1.829853
130	C	20.340250	-1.815765	-0.063071
131	C	20.931571	2.714660	1.101144
132	C	21.003438	2.842253	-0.375057
133	C	21.830425	-1.787963	0.012391
134	C	19.928556	-1.131569	-1.277967
135	C	19.768005	2.307373	-0.917718
136	C	22.211266	-1.333221	1.342248
137	C	22.196689	2.156021	1.572768
138	C	19.806007	-1.345750	1.205427
139	C	22.334785	-1.116146	-1.177338
140	C	19.654097	2.105886	1.422330
141	C	22.313553	2.361815	-0.809840
142	C	18.303601	0.504123	0.036419
143	C	20.903958	0.244499	2.575858
144	C	21.140069	0.659593	-2.244643
145	C	23.492404	0.594885	0.298874
146	U	-14.047148	-0.086025	0.063519
147	C	-16.264854	-1.366133	-0.040549
148	C	-13.989618	1.266108	2.118911
149	C	-12.097645	-1.748267	0.092943
150	C	-13.850374	1.355565	-1.922613
151	C	-12.008254	0.213887	1.404446
152	C	-15.294836	-0.462321	-1.978877
153	C	-15.990966	0.643026	-1.250936
154	C	-12.896749	-0.782790	2.078796
155	C	-11.922428	0.269238	-1.120197
156	C	-16.079063	0.587937	1.273129
157	C	-15.432631	-0.549886	1.996871
158	C	-12.760095	-0.695088	-1.897009
159	C	-13.090115	2.132966	0.145539
160	C	-14.281532	-2.400331	0.743576

161	C	-14.231312	-2.368515	-0.731715
162	C	-14.587482	2.270765	0.096700
163	C	-12.656754	1.505573	-1.094173
164	C	-12.901324	-1.890157	-1.100376
165	C	-15.132916	1.670520	1.305085
166	C	-15.505469	-1.708992	1.141058
167	C	-12.741679	1.450450	1.382922
168	C	-15.047607	1.725354	-1.171964
169	C	-12.979977	-1.941147	1.222824
170	C	-15.425727	-1.658448	-1.182100
171	C	-11.313796	-0.404741	0.149954
172	C	-14.129220	-0.121449	2.479293
173	C	-13.962445	-0.015236	-2.351530
174	C	-16.792469	0.098422	-0.027846
175	U	-21.040798	0.795935	-0.047945
176	C	-23.089931	0.455192	-1.355449
177	C	-21.197935	-0.321084	2.142717
178	C	-19.062979	-0.221277	-1.330463
179	C	-20.595716	3.198132	0.278116
180	C	-19.155117	-0.408262	1.009732
181	C	-21.986768	2.502085	-1.464339
182	C	-22.759532	2.458815	-0.203124
183	C	-20.069553	-1.396329	0.422828
184	C	-18.779917	1.792344	-0.156514
185	C	-23.138955	0.244132	0.969600
186	C	-22.586053	-1.000568	0.391184
187	C	-19.475394	2.078329	-1.417699
188	C	-20.106807	1.717784	1.994105
189	C	-21.248099	-0.917201	-1.746254
190	C	-21.026884	0.379326	-2.432948
191	C	-21.579050	1.962206	1.978940
192	C	-19.505958	2.463852	0.899704
193	C	-19.671609	0.803141	-2.133011
194	C	-22.256119	0.675629	2.066354
195	C	-22.539500	-0.855574	-1.064544
196	C	-19.879013	0.282549	2.054908
197	C	-21.877120	2.888734	0.894833
198	C	-20.022516	-1.251552	-1.044223
199	C	-22.182065	1.236727	-2.173135
200	C	-18.307063	0.309256	-0.082878
201	C	-21.345425	-1.314224	1.102144
202	C	-20.621115	2.917821	-1.140104
203	C	-23.431879	1.162355	-0.130330

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
$(U@C_{28})_7$-triplet	1	U	-0.000423	-0.661842	0.012689
	2	C	-2.062360	-2.136072	0.379175
	3	C	-0.123427	0.358600	-2.222857
	4	C	0.069876	1.077426	1.751688
	5	C	2.116860	-2.094123	0.169098
	6	C	0.707258	1.606804	-0.432053
	7	C	0.077939	-2.803072	1.147289
	8	C	0.007851	-3.065452	-0.304248
	9	C	-0.794583	1.591760	-0.356223
	10	C	2.092638	0.090654	1.059377
	11	C	-1.357526	-1.559133	-1.783521
	12	C	-2.112786	-0.399107	-1.216579
	13	C	1.376955	-0.826186	1.999970
	14	C	1.972181	-0.357369	-1.422454
	15	C	-1.992587	0.050472	1.264900
	16	C	-1.168094	-0.851298	2.127841
	17	C	1.187384	-1.533038	-1.911675
	18	C	2.751312	-0.702928	-0.113695
	19	C	0.114491	-0.215546	2.385351
	20	C	-0.115992	-1.074860	-2.366005
	21	C	-2.749562	-0.757634	0.163639
	22	C	1.108952	0.784036	-1.563811
	23	C	1.243306	-2.549779	-0.888999
	24	C	-1.172998	1.200513	0.993911
	25	C	-1.179683	-2.162004	1.523875
	26	C	1.227491	1.224470	0.872766
	27	C	-1.291440	0.759716	-1.442481
	28	C	1.353706	-2.136732	1.396291
	29	C	-1.289985	-2.575399	-0.761265
	30	U	7.019451	-0.360484	-0.224275
	31	C	9.146094	-1.123379	-1.429379
	32	C	6.818245	2.084881	-0.408136
	33	C	4.976775	-1.456917	-1.312305
	34	C	7.140369	-1.040540	2.137468
	35	C	4.866630	0.776472	-0.560879
	36	C	8.462424	-2.136519	0.573924
	37	C	9.143312	-0.848513	0.913863
	38	C	5.607074	0.736171	-1.859932
	39	C	5.066877	-1.174422	1.029064
	40	C	8.942045	1.103477	-0.675111
	41	C	8.146045	0.939638	-1.930995
	42	C	5.923270	-2.339368	0.645501
	43	C	6.204558	1.025764	1.581122
	44	C	7.026622	-1.243635	-2.482234
	45	C	7.143885	-2.384944	-1.552569

46	C	7.702977	1.145833	1.538945
47	C	5.872551	-0.356468	1.894962
48	C	5.897026	-2.443955	-0.793672
49	C	8.070173	1.751510	0.267130
50	C	8.239899	-0.444567	-2.328387
51	C	5.675118	1.559352	0.334472
52	C	8.267668	-0.164596	1.827248
53	C	5.712382	-0.647086	-2.257403
54	C	8.424499	-2.241653	-0.864835
55	C	4.277175	-0.624273	-0.200847
56	C	6.826596	1.518228	-1.732598
57	C	7.211090	-2.218060	1.310464
58	C	9.765373	-0.184305	-0.355894
59	U	-7.028544	-0.564454	0.172738
60	C	-9.134331	-0.953983	1.576684
61	C	-6.924486	1.803257	-0.488602
62	C	-4.954543	-1.142510	1.559070
63	C	-7.102187	-2.012627	-1.815118
64	C	-4.924233	0.703825	0.090925
65	C	-8.394679	-2.561206	0.034743
66	C	-9.121694	-1.494054	-0.720665
67	C	-5.674112	1.079154	1.329715
68	C	-5.035116	-1.678414	-0.737736
69	C	-9.010599	0.888234	0.108247
70	C	-8.219675	1.193985	1.340501
71	C	-5.848820	-2.676029	0.023961
72	C	-6.252518	0.155056	-2.001022
73	C	-7.020982	-0.624651	2.596658
74	C	-7.085923	-2.018155	2.112117
75	C	-7.754853	0.222845	-1.994635
76	C	-5.864211	-1.237062	-1.826550
77	C	-5.831133	-2.282751	1.412467
78	C	-8.156497	1.210256	-1.003305
79	C	-8.262865	0.025315	2.185990
80	C	-5.755170	1.102006	-1.013486
81	C	-8.265432	-1.128782	-1.816654
82	C	-5.729086	-0.088907	2.175347
83	C	-8.365342	-2.168576	1.423240
84	C	-4.277931	-0.711778	0.227103
85	C	-6.922078	1.722038	0.949705
86	C	-7.134561	-2.839655	-0.635894
87	C	-9.780403	-0.463207	0.250007
88	U	14.027913	0.196094	-0.176986
89	C	16.115538	0.926001	-1.467449
90	C	13.823680	1.553358	1.865336
91	C	11.952032	0.550552	-1.633632
92	C	14.221143	-2.190465	0.389503

93	C	11.866496	0.991544	0.682509
94	C	15.493215	-1.333532	-1.354311
95	C	16.185194	-0.978326	-0.076478
96	C	12.566906	2.121827	-0.002954
97	C	12.114606	-1.345979	-0.238604
98	C	15.936816	1.359356	0.845466
99	C	15.102722	2.350795	0.098346
100	C	12.957435	-1.562469	-1.455130
101	C	13.270540	-0.715038	1.930503
102	C	13.964883	1.727715	-2.055555
103	C	14.109583	0.360593	-2.594571
104	C	14.767058	-0.579597	1.990411
105	C	12.947105	-1.676542	0.886404
106	C	12.886742	-0.361877	-2.253023
107	C	15.095381	0.834730	1.886732
108	C	15.183089	2.018537	-1.303695
109	C	12.703318	0.618430	1.791051
110	C	15.339078	-1.460068	0.982059
111	C	12.658706	1.790631	-1.404511
112	C	15.410890	-0.134140	-2.152407
113	C	11.287550	-0.026220	-0.351349
114	C	13.790495	2.427731	0.720918
115	C	14.265181	-2.047838	-1.043402
116	C	16.768473	0.469734	-0.132209
117	U	21.056013	0.604027	0.235688
118	C	22.995444	2.110525	0.204896
119	C	20.856914	-0.527726	2.415055
120	C	18.928159	1.989500	-0.148630
121	C	21.219123	-1.075294	-1.559855
122	C	18.897375	0.199922	1.369794
123	C	22.446487	0.905475	-1.710448
124	C	23.141843	-0.003825	-0.774307
125	C	19.551281	1.347528	2.011174
126	C	19.123357	-0.142534	-1.112550
127	C	22.914209	0.340463	1.725079
128	C	22.086399	1.450266	2.244392
129	C	19.908311	0.806900	-1.911526
130	C	20.320176	-1.694916	0.485179
131	C	20.881569	2.985313	0.643424
132	C	21.014657	2.783529	-0.819761
133	C	21.804917	-1.644692	0.613671
134	C	19.960968	-1.296251	-0.867060
135	C	19.799128	2.137633	-1.281727
136	C	22.133022	-0.904133	1.824500
137	C	22.123711	2.549914	1.278196
138	C	19.736592	-0.956941	1.594869
139	C	22.360640	-1.248201	-0.673310

140	C	19.588124	2.457376	1.038536
141	C	22.338640	2.224526	-1.083834
142	C	18.289479	0.581752	-0.013474
143	C	20.783622	0.901118	2.624717
144	C	21.218840	0.242798	-2.154404
145	C	23.464780	0.752263	0.434757
146	U	-14.038951	-0.036156	0.076912
147	C	-16.270844	-1.278259	0.252966
148	C	-13.939770	1.698729	1.818806
149	C	-12.110718	-1.685574	0.420588
150	C	-13.849560	0.974422	-2.158354
151	C	-11.979903	0.496414	1.310001
152	C	-15.317415	-0.796422	-1.836520
153	C	-15.991326	0.442207	-1.337989
154	C	-12.871452	-0.331555	2.179965
155	C	-11.923822	0.043650	-1.173075
156	C	-16.047773	0.894135	1.145485
157	C	-15.405621	-0.083842	2.077758
158	C	-12.783376	-1.044704	-1.734122
159	C	-13.054572	2.140188	-0.297141
160	C	-14.293017	-2.164836	1.209472
161	C	-14.260465	-2.429347	-0.242955
162	C	-14.550092	2.286556	-0.357759
163	C	-12.642944	1.270262	-1.389458
164	C	-12.929349	-2.053547	-0.712671
165	C	-15.088707	1.948246	0.951598
166	C	-15.503079	-1.390159	1.472573
167	C	-12.698418	1.714371	1.048621
168	C	-15.033393	1.504424	-1.486269
169	C	-12.980635	-1.636933	1.574081
170	C	-15.451669	-1.806398	-0.814460
171	C	-11.307305	-0.372698	0.200464
172	C	-14.090917	0.413148	2.451265
173	C	-13.983532	-0.452585	-2.303375
174	C	-16.784506	0.163340	-0.022004
175	U	-21.033320	0.858118	-0.080348
176	C	-23.118051	0.249912	-1.227012
177	C	-21.123805	0.228958	2.299994
178	C	-19.088160	-0.411227	-1.175286
179	C	-20.590450	3.273275	-0.284259
180	C	-19.114744	-0.096827	1.151287
181	C	-22.027975	2.226771	-1.798092
182	C	-22.763935	2.451461	-0.535401
183	C	-20.039708	-1.186335	0.814751
184	C	-18.781521	1.804093	-0.463016
185	C	-23.099219	0.537211	1.089741
186	C	-22.558410	-0.802308	0.773305

	187	C	-19.513796	1.817864	-1.735770
	188	C	-20.047676	2.190457	1.692385
	189	C	-21.281557	-1.175625	-1.371810
	190	C	-21.085521	-0.054955	-2.323161
	191	C	-21.519600	2.428162	1.668596
	192	C	-19.480884	2.685192	0.447229
	193	C	-19.723180	0.419659	-2.160203
	194	C	-22.187500	1.189441	2.044895
	195	C	-22.552936	-0.970010	-0.681453
	196	C	-19.811350	0.799734	2.047755
	197	C	-21.852318	3.102255	0.420863
	198	C	-20.034012	-1.357397	-0.651593
	199	C	-22.236192	0.839139	-2.217016
	200	C	-18.298717	0.369595	-0.091535
	201	C	-21.295949	-0.961466	1.497444
	202	C	-20.654931	2.698996	-1.609704
	203	C	-23.428609	1.201245	-0.170582

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
(a)	1	U	0.167066	2.986053	0.088805
	2	C	-1.999320	1.816195	0.373379
	3	C	0.765820	4.137105	2.196318
	4	C	1.923386	1.333022	-0.476544
	5	C	-0.024332	4.644335	-1.737470
	6	C	2.429722	3.098166	0.948177
	7	C	-1.524756	2.870557	-1.643156
	8	C	-1.947685	3.893963	-0.668269
	9	C	1.709101	2.066361	1.718221
	10	C	1.935981	3.414962	-1.509994
	11	C	-1.453784	3.577067	1.789773
	12	C	-0.742751	2.368539	2.249553
	13	C	0.926713	2.568040	-2.174178
	14	C	1.212005	5.168831	0.160638
	15	C	-0.019057	0.612938	0.579700
	16	C	-0.307102	0.799850	-0.855294
	17	C	-0.219694	5.345102	0.471037
	18	C	1.331906	4.718290	-1.227328
	19	C	0.915446	1.259203	-1.517566
	20	C	-0.500112	4.687125	1.748919
	21	C	-1.080473	1.263557	1.350842
	22	C	1.828318	4.399817	1.243691
	23	C	-0.996659	5.005468	-0.722600
	24	C	1.384700	0.958517	0.817712

25	C	-1.550316	1.563260	-0.982982
26	C	2.556666	2.636817	-0.435676
27	C	0.656659	2.721827	2.496397
28	C	-0.308757	3.341213	-2.308208
29	C	-2.237554	3.228524	0.603427
30	U	-3.735185	-3.612324	0.397792
31	C	-5.051122	-4.372372	2.350553
32	C	-2.984093	-1.281373	0.765173
33	C	-1.755933	-5.077185	0.113884
34	C	-5.137154	-3.715473	-1.638859
35	C	-1.545967	-2.791249	-0.262841
36	C	-5.708107	-5.003046	0.211262
37	C	-6.155769	-3.617264	0.449085
38	C	-1.517027	-3.031337	1.192651
39	C	-2.894212	-4.314898	-1.764519
40	C	-4.809058	-2.094610	1.951617
41	C	-3.575499	-2.591561	2.590619
42	C	-3.648646	-5.443458	-1.186302
43	C	-3.660843	-1.941250	-1.357637
44	C	-2.809008	-4.964403	2.183370
45	C	-3.594653	-5.853837	1.306823
46	C	-4.862933	-1.684205	-0.541417
47	C	-3.832265	-3.224900	-2.040584
48	C	-2.934357	-5.915957	0.001136
49	C	-4.433652	-1.275006	0.797180
50	C	-3.726869	-4.027157	2.832351
51	C	-2.478802	-1.694755	-0.530214
52	C	-5.787326	-2.806466	-0.713434
53	C	-1.654974	-4.470387	1.428623
54	C	-5.004618	-5.473042	1.406253
55	C	-1.708595	-4.080431	-0.938752
56	C	-2.426457	-2.083338	1.837646
57	C	-5.059078	-5.060463	-1.100110
58	C	-5.732617	-3.219182	1.792899
59	U	3.839100	-3.745513	-0.107487
60	C	2.915508	-5.805236	0.910572
61	C	5.430928	-2.686893	1.464661
62	C	5.006727	-4.314266	-2.213191
63	C	1.985075	-2.165254	-0.592108
64	C	5.900454	-2.688225	-0.812422
65	C	1.525725	-4.431321	-0.347796
66	C	1.680154	-3.837829	0.993754
67	C	6.239444	-4.015449	-0.264321
68	C	3.748007	-2.362429	-2.097252
69	C	3.830309	-4.163351	2.279301
70	C	4.931822	-4.946919	1.688169
71	C	2.830305	-3.499846	-2.299181

	72	C	4.013210	-1.346204	0.200604
	73	C	4.667054	-5.964234	-0.610452
	74	C	3.410792	-5.774142	-1.360741
	75	C	3.249903	-1.889413	1.339936
	76	C	3.219098	-1.529012	-1.016178
	77	C	3.624416	-4.728091	-2.362505
	78	C	4.142156	-2.740718	2.128923
	79	C	4.353724	-5.974702	0.819805
	80	C	5.382849	-1.856644	0.275855
	81	C	1.976893	-2.411933	0.838371
	82	C	5.668165	-5.038076	-1.143281
	83	C	2.310834	-5.664829	-0.400809
	84	C	5.116588	-2.878776	-2.034259
	85	C	5.934103	-4.015289	1.167728
	86	C	1.726444	-3.378223	-1.344939
	87	C	2.562034	-4.699613	1.781373

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
(b)	1	U	-1.685983	3.770427	0.009806
	2	C	-2.052453	5.876957	-1.195487
	3	C	0.722062	3.339444	0.315048
	4	C	-2.806173	3.804542	2.203431
	5	C	-2.677627	1.843835	-1.370409
	6	C	-0.751473	2.748749	2.004832
	7	C	-3.399988	4.039195	-1.678916
	8	C	-2.101199	3.867861	-2.374082
	9	C	-0.526264	4.221732	2.062883
	10	C	-2.864952	1.820640	0.969626
	11	C	0.009505	4.806159	-1.356382
	12	C	-0.045124	5.514843	-0.059152
	13	C	-3.865270	2.749343	0.428891
	14	C	-0.662341	1.532304	-0.209228
	15	C	-2.264096	5.807776	1.128428
	16	C	-3.501492	5.269392	0.523079
	17	C	-0.383300	2.289828	-1.435061
	18	C	-2.137107	1.033918	-0.161906
	19	C	-3.800495	3.990777	1.170278
	20	C	0.441415	3.431065	-1.100706
	21	C	-1.349739	6.167072	0.045355
	22	C	0.002236	2.211010	0.882401
	23	C	-1.660947	2.503515	-2.142937
	24	C	-1.822105	4.876887	2.180741
	25	C	-3.356037	5.295785	-0.933865
	26	C	-2.183977	2.499723	2.050805
	27	C	0.395083	4.584294	0.994041
	28	C	-3.719588	2.775587	-1.039524
	29	C	-1.259438	5.018757	-2.055387

30	U	-2.750963	-3.223599	0.009530
31	C	-2.228891	-5.339888	-1.121025
32	C	-1.851752	-3.208013	2.304030
33	C	-1.656636	-1.299376	-1.295248
34	C	-5.182083	-2.832998	0.067680
35	C	-1.703207	-1.240344	1.051403
36	C	-4.282240	-4.309487	-1.501794
37	C	-4.345103	-4.999429	-0.195139
38	C	-0.640305	-2.158929	0.626624
39	C	-3.784380	-1.005459	-0.344725
40	C	-2.250692	-5.235101	1.211161
41	C	-0.968462	-4.682602	0.723176
42	C	-3.925726	-1.787695	-1.579482
43	C	-3.893638	-2.192829	1.885461
44	C	-0.870660	-3.485190	-1.496492
45	C	-2.096746	-3.346940	-2.319491
46	C	-4.099019	-3.668791	1.943803
47	C	-4.539725	-1.684961	0.685270
48	C	-2.580463	-1.987885	-2.153316
49	C	-2.810601	-4.298286	2.199904
50	C	-0.967807	-4.731293	-0.740202
51	C	-2.477195	-1.917029	2.070012
52	C	-4.903618	-4.063000	0.794940
53	C	-0.637171	-2.207681	-0.848592
54	C	-2.946950	-4.508373	-2.068634
55	C	-2.328014	-0.482777	-0.159272
56	C	-0.756761	-3.390292	1.377240
57	C	-4.760984	-2.938913	-1.311542
58	C	-3.046406	-5.625934	0.048327
59	U	4.437336	-0.546438	0.000405
60	C	4.963360	1.722925	-0.839015
61	C	6.384170	-2.032387	-0.351856
62	C	3.909175	-0.430867	2.417738
63	C	2.479286	-1.444709	-1.226918
64	C	5.131827	-2.230511	1.596878
65	C	2.831178	0.852679	-1.162992
66	C	3.734350	0.268195	-2.172451
67	C	6.038029	-1.074914	1.738398
68	C	2.692506	-1.863220	1.049599
69	C	6.174963	-0.098733	-1.626366
70	C	6.697150	0.271171	-0.296861
71	C	2.174627	-0.493776	0.871569
72	C	4.237551	-2.864114	-0.680647
73	C	5.150035	1.271659	1.434061
74	C	3.725790	1.485639	1.114525
75	C	4.622165	-2.078253	-1.868242
76	C	2.889477	-2.459574	-0.273740

	77	C	2.945891	0.408532	1.727980
	78	C	5.969709	-1.548066	-1.655062
	79	C	5.926490	1.412471	0.200772
	80	C	5.344908	-2.826614	0.276581
	81	C	3.516394	-1.179344	-2.206116
	82	C	5.264128	0.059099	2.247080
	83	C	3.609797	1.761059	-0.318312
	84	C	3.790472	-1.820408	2.016825
	85	C	6.819609	-0.946668	0.506805
	86	C	2.049679	-0.229659	-0.562068
	87	C	5.077422	0.810912	-1.961732

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
(c)	1	U	-0.135708	3.167894	-1.189237
	2	C	-2.134247	1.941839	-0.386568
	3	C	0.297808	5.102716	0.292454
	4	C	1.826062	1.651111	-1.160446
	5	C	-0.527454	3.964470	-3.499500
	6	C	2.088181	3.875590	-0.539064
	7	C	-1.786935	2.193797	-2.671928
	8	C	-2.344550	3.452902	-2.141880
	9	C	1.502508	3.137594	0.596266
	10	C	1.574162	3.164460	-2.908036
	11	C	-1.828648	4.163816	0.228054
	12	C	-0.970412	3.319646	1.081167
	13	C	0.686806	2.011517	-3.155392
	14	C	0.618959	5.321906	-1.999998
	15	C	-0.015200	1.162844	0.173286
	16	C	-0.316255	0.747897	-1.210136
	17	C	-0.825276	5.427915	-1.717567
	18	C	0.804658	4.392819	-3.116337
	19	C	0.840442	1.064597	-2.049807
	20	C	-1.025807	5.280183	-0.274625
	21	C	-1.157718	1.921598	0.687040
	22	C	1.323298	5.108041	-0.734267
	23	C	-1.544609	4.565655	-2.657237
	24	C	1.331679	1.738212	0.201542
	25	C	-1.646133	1.247917	-1.563686
	26	C	2.282560	2.938606	-1.647139
	27	C	0.370363	3.907518	1.112655
	28	C	-0.637546	2.518007	-3.518834
	29	C	-2.553184	3.294930	-0.701417
	30	U	-3.414003	-3.254115	1.458462
	31	C	-4.198195	-4.091570	3.650482
	32	C	-2.372653	-1.024008	1.750299

33	C	-1.737392	-4.825745	0.524808
34	C	-5.330215	-3.073604	-0.096230
35	C	-1.428806	-2.536760	0.257530
36	C	-5.481716	-4.478389	1.750527
37	C	-5.713036	-3.091243	2.197367
38	C	-1.018277	-2.908107	1.624850
39	C	-3.277237	-3.817650	-0.895381
40	C	-3.864365	-1.809910	3.350723
41	C	-2.554206	-2.449360	3.577331
42	C	-3.943259	-4.936750	-0.202285
43	C	-3.674196	-1.442004	-0.130870
44	C	-2.157361	-4.824946	2.811692
45	C	-3.236113	-5.573041	2.138549
46	C	-4.571649	-1.173797	1.009430
47	C	-4.148452	-2.643400	-0.819732
48	C	-2.973895	-5.564691	0.697798
49	C	-3.749968	-0.918268	2.194431
50	C	-2.765885	-3.886778	3.756285
51	C	-2.291823	-1.359477	0.341638
52	C	-5.608224	-2.207301	1.034583
53	C	-1.218241	-4.349101	1.793378
54	C	-4.520006	-5.102951	2.661176
55	C	-1.890134	-3.744714	-0.431130
56	C	-1.618376	-1.959451	2.563104
57	C	-5.231127	-4.463301	0.307963
58	C	-4.897071	-2.846981	3.388447
59	U	3.839526	-3.417423	-0.799736
60	C	2.680402	-5.550000	-1.287423
61	C	5.632434	-3.808904	0.859450
62	C	4.819702	-2.510875	-2.883286
63	C	2.207068	-1.784331	0.120174
64	C	5.996297	-2.316680	-0.886614
65	C	1.442932	-3.587663	-1.135409
66	C	1.740114	-4.060602	0.229490
67	C	6.167835	-3.689754	-1.400152
68	C	3.855337	-1.054239	-1.349349
69	C	3.877923	-5.324837	0.692610
70	C	4.830658	-5.589319	-0.403035
71	C	2.778521	-1.689978	-2.131540
72	C	4.362429	-1.865577	0.988310
73	C	4.322367	-4.778243	-2.742214
74	C	3.073192	-4.040577	-3.011908
75	C	3.582268	-2.972798	1.571217
76	C	3.498112	-1.119287	0.070780
77	C	3.387153	-2.612792	-3.090029
78	C	4.379991	-4.197248	1.479367
79	C	4.074893	-5.721952	-1.650067

	80	C	5.649486	-2.394757	0.534617
	81	C	2.228246	-2.925449	1.015778
	82	C	5.418688	-3.812197	-2.651815
	83	C	2.043697	-4.521172	-2.088406
	84	C	5.138254	-1.579891	-1.816892
	85	C	5.930164	-4.627877	-0.301082
	86	C	1.743241	-2.155163	-1.204673
	87	C	2.526168	-5.290652	0.131756
	88	U	7.161952	3.010123	1.033772
	89	C	6.355215	0.675421	1.198224
	90	C	7.882358	3.792243	3.268762
	91	C	9.071805	3.113579	-0.536583
	92	C	5.328771	4.455989	0.203265
	93	C	9.100456	4.416344	1.389189
	94	C	5.246497	2.166655	-0.198589
	95	C	4.812289	2.413493	1.189810
	96	C	9.474570	3.036028	1.752341
	97	C	7.504445	4.830872	-0.526485
	98	C	6.409822	1.999988	3.105320
	99	C	7.775414	1.510508	2.835793
	100	C	6.946701	3.692490	-1.281529
	101	C	6.761351	5.255179	1.851269
	102	C	8.518678	1.085987	0.457803
	103	C	7.587350	1.328266	-0.660659
	104	C	5.769959	4.363930	2.483921
	105	C	6.486973	5.304075	0.413860
	106	C	7.931737	2.609386	-1.278745
	107	C	6.479071	3.438130	3.368569
	108	C	7.739160	0.681078	1.629532
	109	C	8.091587	4.887466	2.339938
	110	C	4.875184	3.854773	1.443619
	111	C	9.446190	2.215506	0.539695
	112	C	6.223585	1.075790	-0.190250
	113	C	8.838662	4.460988	-0.050761
	114	C	8.699174	2.641954	2.930152
	115	C	5.579956	3.452697	-0.814573
	116	C	5.516940	1.476983	2.068396

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
(d)	1	U	-0.135708	3.167894	-1.189237
	2	C	-2.134247	1.941839	-0.386568
	3	C	0.297808	5.102716	0.292454
	4	C	1.826062	1.651111	-1.160446
	5	C	-0.527454	3.964470	-3.499500
	6	C	2.088181	3.875590	-0.539064

7	C	-1.786935	2.193797	-2.671928
8	C	-2.344550	3.452902	-2.141880
9	C	1.502508	3.137594	0.596266
10	C	1.574162	3.164460	-2.908036
11	C	-1.828648	4.163816	0.228054
12	C	-0.970412	3.319646	1.081167
13	C	0.686806	2.011517	-3.155392
14	C	0.618959	5.321906	-1.999998
15	C	-0.015200	1.162844	0.173286
16	C	-0.316255	0.747897	-1.210136
17	C	-0.825276	5.427915	-1.717567
18	C	0.804658	4.392819	-3.116337
19	C	0.840442	1.064597	-2.049807
20	C	-1.025807	5.280183	-0.274625
21	C	-1.157718	1.921598	0.687040
22	C	1.323298	5.108041	-0.734267
23	C	-1.544609	4.565655	-2.657237
24	C	1.331679	1.738212	0.201542
25	C	-1.646133	1.247917	-1.563686
26	C	2.282560	2.938606	-1.647139
27	C	0.370363	3.907518	1.112655
28	C	-0.637546	2.518007	-3.518834
29	C	-2.553184	3.294930	-0.701417
30	U	-3.414003	-3.254115	1.458462
31	C	-4.198195	-4.091570	3.650482
32	C	-2.372653	-1.024008	1.750299
33	C	-1.737392	-4.825745	0.524808
34	C	-5.330215	-3.073604	-0.096230
35	C	-1.428806	-2.536760	0.257530
36	C	-5.481716	-4.478389	1.750527
37	C	-5.713036	-3.091243	2.197367
38	C	-1.018277	-2.908107	1.624850
39	C	-3.277237	-3.817650	-0.895381
40	C	-3.864365	-1.809910	3.350723
41	C	-2.554206	-2.449360	3.577331
42	C	-3.943259	-4.936750	-0.202285
43	C	-3.674196	-1.442004	-0.130870
44	C	-2.157361	-4.824946	2.811692
45	C	-3.236113	-5.573041	2.138549
46	C	-4.571649	-1.173797	1.009430
47	C	-4.148452	-2.643400	-0.819732
48	C	-2.973895	-5.564691	0.697798
49	C	-3.749968	-0.918268	2.194431
50	C	-2.765885	-3.886778	3.756285
51	C	-2.291823	-1.359477	0.341638
52	C	-5.608224	-2.207301	1.034583
53	C	-1.218241	-4.349101	1.793378

54	C	-4.520006	-5.102951	2.661176
55	C	-1.890134	-3.744714	-0.431130
56	C	-1.618376	-1.959451	2.563104
57	C	-5.231127	-4.463301	0.307963
58	C	-4.897071	-2.846981	3.388447
59	U	3.839526	-3.417423	-0.799736
60	C	2.680402	-5.550000	-1.287423
61	C	5.632434	-3.808904	0.859450
62	C	4.819702	-2.510875	-2.883286
63	C	2.207068	-1.784331	0.120174
64	C	5.996297	-2.316680	-0.886614
65	C	1.442932	-3.587663	-1.135409
66	C	1.740114	-4.060602	0.229490
67	C	6.167835	-3.689754	-1.400152
68	C	3.855337	-1.054239	-1.349349
69	C	3.877923	-5.324837	0.692610
70	C	4.830658	-5.589319	-0.403035
71	C	2.778521	-1.689978	-2.131540
72	C	4.362429	-1.865577	0.988310
73	C	4.322367	-4.778243	-2.742214
74	C	3.073192	-4.040577	-3.011908
75	C	3.582268	-2.972798	1.571217
76	C	3.498112	-1.119287	0.070780
77	C	3.387153	-2.612792	-3.090029
78	C	4.379991	-4.197248	1.479367
79	C	4.074893	-5.721952	-1.650067
80	C	5.649486	-2.394757	0.534617
81	C	2.228246	-2.925449	1.015778
82	C	5.418688	-3.812197	-2.651815
83	C	2.043697	-4.521172	-2.088406
84	C	5.138254	-1.579891	-1.816892
85	C	5.930164	-4.627877	-0.301082
86	C	1.743241	-2.155163	-1.204673
87	C	2.526168	-5.290652	0.131756
88	U	7.161952	3.010123	1.033772
89	C	6.355215	0.675421	1.198224
90	C	7.882358	3.792243	3.268762
91	C	9.071805	3.113579	-0.536583
92	C	5.328771	4.455989	0.203265
93	C	9.100456	4.416344	1.389189
94	C	5.246497	2.166655	-0.198589
95	C	4.812289	2.413493	1.189810
96	C	9.474570	3.036028	1.752341
97	C	7.504445	4.830872	-0.526485
98	C	6.409822	1.999988	3.105320
99	C	7.775414	1.510508	2.835793
100	C	6.946701	3.692490	-1.281529

	101	C	6.761351	5.255179	1.851269
	102	C	8.518678	1.085987	0.457803
	103	C	7.587350	1.328266	-0.660659
	104	C	5.769959	4.363930	2.483921
	105	C	6.486973	5.304075	0.413860
	106	C	7.931737	2.609386	-1.278745
	107	C	6.479071	3.438130	3.368569
	108	C	7.739160	0.681078	1.629532
	109	C	8.091587	4.887466	2.339938
	110	C	4.875184	3.854773	1.443619
	111	C	9.446190	2.215506	0.539695
	112	C	6.223585	1.075790	-0.190250
	113	C	8.838662	4.460988	-0.050761
	114	C	8.699174	2.641954	2.930152
	115	C	5.579956	3.452697	-0.814573
	116	C	5.516940	1.476983	2.068396

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
(e)	1	U	0.017451	10.625605	-0.110002
	2	C	-0.954208	12.817051	-1.007213
	3	C	-0.126544	10.620663	2.345604
	4	C	-1.325948	8.649330	-1.037458
	5	C	2.359206	10.421558	-0.837956
	6	C	-0.535953	8.611964	1.186710
	7	C	0.930932	11.835353	-2.001541
	8	C	1.379365	12.561568	-0.772827
	9	C	-1.741574	9.493970	1.113815
	10	C	1.016481	8.486914	-0.800379
	11	C	-0.172279	12.685825	1.215763
	12	C	-1.515021	12.032315	1.132084
	13	C	0.705025	9.297508	-2.018566
	14	C	1.751293	9.705644	1.300985
	15	C	-2.246374	10.832373	-0.953593
	16	C	-1.338639	10.759873	-2.115881
	17	C	1.884921	11.203589	1.311540
	18	C	1.989689	9.242306	-0.058281
	19	C	-0.729603	9.433391	-2.094711
	20	C	0.679826	11.758515	1.910375
	21	C	-1.933951	12.072840	-0.248433
	22	C	0.465862	9.364171	1.893021
	23	C	2.203175	11.636428	-0.041569
	24	C	-2.158992	9.545823	-0.266723
	25	C	-0.505024	11.958069	-2.079674
	26	C	-0.281848	7.886721	-0.172782
	27	C	-1.455266	10.743053	1.802326

28	C	1.516380	10.504384	-2.003422
29	C	0.206706	13.372666	-0.134848
30	U	0.878467	17.625498	-0.082541
31	C	-0.143351	19.778520	0.510375
32	C	2.934568	17.240209	1.219124
33	C	-0.782913	15.745031	0.463429
34	C	1.390149	17.528977	-2.490609
35	C	1.509778	15.424472	0.849965
36	C	-0.192144	19.054509	-1.702193
37	C	1.155897	19.593426	-1.420452
38	C	0.962386	16.249073	1.934757
39	C	0.545887	15.605015	-1.467154
40	C	2.127062	19.411943	0.912333
41	C	1.344642	18.767632	1.988902
42	C	-0.561621	16.533487	-1.726402
43	C	2.848043	16.534391	-0.987342
44	C	-0.945711	17.827503	1.498153
45	C	-1.514225	17.933474	0.132632
46	C	3.076175	18.007940	-0.967594
47	C	1.762442	16.248570	-1.912692
48	C	-1.374744	16.633255	-0.498194
49	C	3.122207	18.443507	0.421690
50	C	-0.078952	18.982532	1.721545
51	C	2.718707	16.069631	0.385152
52	C	2.151738	18.624957	-1.909308
53	C	-0.473200	16.465139	1.667244
54	C	-0.996893	19.153721	-0.482735
55	C	0.387871	14.891116	-0.091171
56	C	1.826231	17.392762	2.135143
57	C	-0.030838	17.739455	-2.325202
58	C	1.187155	20.026440	-0.024166
59	U	-0.307873	-3.449196	0.016349
60	C	-1.448266	-1.413736	-1.055886
61	C	-0.689086	-3.355880	2.448639
62	C	-1.274295	-5.492508	-0.944127
63	C	2.107559	-3.315562	-0.451148
64	C	-0.744558	-5.405991	1.327869
65	C	0.643869	-2.134112	-1.809748
66	C	0.850380	-1.349645	-0.585748
67	C	-2.036991	-4.719523	1.115582
68	C	1.014027	-5.380695	-0.495515
69	C	-0.895832	-1.374996	1.225683
70	C	-2.115823	-2.173552	1.052005
71	C	0.745552	-4.679648	-1.769434
72	C	1.369348	-4.046242	1.625543
73	C	-2.481455	-3.503130	-1.050874
74	C	-1.452144	-3.488462	-2.118189

75	C	1.310120	-2.556725	1.589176
76	C	1.864570	-4.514387	0.338132
77	C	-0.693213	-4.734484	-2.036281
78	C	0.002143	-2.135928	2.066802
79	C	-2.438567	-2.212056	-0.388039
80	C	0.107275	-4.539766	2.160196
81	C	1.734198	-2.110787	0.270873
82	C	-2.355046	-4.758235	-0.313315
83	C	-0.806131	-2.188877	-2.080775
84	C	-0.260199	-5.870174	0.028649
85	C	-1.969429	-3.416151	1.779195
86	C	1.393082	-3.367939	-1.707213
87	C	-0.470302	-0.678526	-0.101826
88	U	-0.363423	3.602270	-0.142718
89	C	-1.729281	5.728088	0.268892
90	C	1.565821	3.572807	1.383903
91	C	-1.821609	1.546712	0.303816
92	C	0.390325	3.566061	-2.484943
93	C	0.452214	1.547728	0.932237
94	C	-1.430382	4.886337	-1.902482
95	C	-0.191835	5.634154	-1.518974
96	C	-0.328827	2.344889	1.928361
97	C	-0.281158	1.543521	-1.483725
98	C	0.542256	5.637070	0.896771
99	C	-0.272468	4.892250	1.906639
100	C	-1.485412	2.337824	-1.879546
101	C	1.818197	2.796802	-0.804643
102	C	-2.357816	3.658020	1.234342
103	C	-2.786864	3.655738	-0.178714
104	C	1.851215	4.300370	-0.817482
105	C	0.857953	2.359384	-1.807323
106	C	-2.376032	2.373152	-0.744416
107	C	1.631249	4.766441	0.544038
108	C	-1.644406	4.912543	1.459187
109	C	1.578297	2.363471	0.564163
110	C	0.910287	4.762599	-1.827222
111	C	-1.700309	2.377211	1.480670
112	C	-2.320338	4.909578	-0.766172
113	C	-0.490929	0.851114	-0.099695
114	C	0.355614	3.606091	2.164914
115	C	-1.049742	3.597619	-2.460229
116	C	-0.370091	6.358272	-0.146161
117	U	-0.589290	7.224058	-6.884694
118	C	-1.049811	5.277467	-5.421624
119	C	-0.105612	9.209895	-5.478860
120	C	1.366149	6.734053	-8.319038
121	C	-2.566591	7.678321	-8.300634

	122	C	1.102542	8.868603	-7.436054
	123	C	-2.288909	5.567130	-7.367089
	124	C	-2.825507	6.470247	-6.330898
	125	C	1.655713	7.992556	-6.385575
	126	C	-0.434882	7.912211	-9.200292
	127	C	-1.287941	7.426149	-4.568700
	128	C	0.145905	7.082410	-4.575657
	129	C	-0.779237	6.477614	-9.179264
	130	C	-1.354505	9.458629	-7.424708
	131	C	1.065854	5.535597	-6.349287
	132	C	0.168417	4.977005	-7.378742
	133	C	-2.236151	8.927332	-6.367668
	134	C	-1.557681	8.665134	-8.637589
	135	C	0.352207	5.739250	-8.614834
	136	C	-1.445729	8.762444	-5.146130
	137	C	0.295249	5.731383	-5.119790
	138	C	-0.011949	9.627374	-6.865121
	139	C	-2.991164	7.800671	-6.918814
	140	C	1.812130	6.647116	-6.941205
	141	C	-1.165327	4.823386	-6.793922
	142	C	0.912354	8.072158	-8.649173
	143	C	0.888153	8.202487	-5.156145
	144	C	-2.117813	6.332107	-8.603414
	145	C	-2.039421	6.291319	-5.108202

Structure	Number	Atom	x (Å)	y (Å)	z (Å)
(f)	1	U	-0.075567	10.694922	-0.188915
	2	C	-1.092675	12.877430	-1.059322
	3	C	-0.086408	10.722045	2.271489
	4	C	-1.467771	8.710586	-1.015331
	5	C	2.223391	10.479060	-1.038651
	6	C	-0.558436	8.699033	1.162589
	7	C	0.735419	11.880585	-2.141056
	8	C	1.250007	12.621205	-0.947666
	9	C	-1.765884	9.581759	1.143449
	10	C	0.883168	8.547676	-0.904636
	11	C	-0.192039	12.772495	1.119416
	12	C	-1.537776	12.119625	1.116706
	13	C	0.506834	9.342888	-2.114272
	14	C	1.731731	9.791244	1.138673
	15	C	-2.381238	10.894666	-0.911039
	16	C	-1.537810	10.806121	-2.119801
	17	C	1.866564	11.288958	1.122796
	18	C	1.895883	9.310379	-0.225542
	19	C	-0.929939	9.477928	-2.116247

20	C	0.695692	11.853070	1.778303
21	C	-2.030494	12.143715	-0.239490
22	C	0.480154	9.459209	1.803842
23	C	2.111481	11.704193	-0.250688
24	C	-2.257781	9.617384	-0.212929
25	C	-0.702287	12.004051	-2.142842
26	C	-0.379204	7.956920	-0.199801
27	C	-1.442419	10.838933	1.799353
28	C	1.318977	10.548706	-2.157827
29	C	0.114182	13.442153	-0.257782
30	U	0.807033	17.691444	-0.282996
31	C	-0.176842	19.856613	0.329303
32	C	2.915143	17.308326	0.933591
33	C	-0.839478	15.826665	0.354295
34	C	1.214418	17.566053	-2.709650
35	C	1.466107	15.497318	0.645422
36	C	-0.324473	19.109104	-1.871000
37	C	1.037276	19.643176	-1.653343
38	C	0.970050	16.336396	1.743580
39	C	0.404403	15.658042	-1.630023
40	C	2.106777	19.481191	0.637633
41	C	1.367729	18.853057	1.753772
42	C	-0.708124	16.590175	-1.851650
43	C	2.730157	16.579327	-1.259424
44	C	-0.946571	17.921089	1.371930
45	C	-1.572506	18.015636	0.030839
46	C	2.966745	18.051653	-1.265648
47	C	1.604322	16.289849	-2.134053
48	C	-1.467239	16.707888	-0.590883
49	C	3.074765	18.501810	0.115473
50	C	-0.064851	19.073252	1.545293
51	C	2.657631	16.130148	0.122411
52	C	2.005980	18.663774	-2.173698
53	C	-0.474492	16.557904	1.535668
54	C	-1.075557	19.226171	-0.619400
55	C	0.301976	14.960230	-0.240684
56	C	1.847712	17.477044	1.894445
57	C	-0.197024	17.786552	-2.485854
58	C	1.130832	20.090942	-0.264608
59	U	-0.315883	-3.373870	0.114375
60	C	-1.648931	-1.366697	-0.780222
61	C	-0.259719	-3.230386	2.572305
62	C	-1.418223	-5.442523	-0.618696
63	C	1.976620	-3.235958	-0.779053
64	C	-0.493878	-5.304462	1.520929
65	C	0.283290	-2.092825	-1.877309
66	C	0.697043	-1.279854	-0.727660

67	C	-1.810049	-4.629978	1.528324
68	C	0.912323	-5.308075	-0.586802
69	C	-0.699385	-1.277710	1.365656
70	C	-1.923152	-2.086444	1.427947
71	C	0.414807	-4.635473	-1.806525
72	C	1.626400	-3.926203	1.410158
73	C	-2.644264	-3.462868	-0.548465
74	C	-1.821340	-3.465444	-1.782131
75	C	1.547229	-2.438039	1.355004
76	C	1.889298	-4.418867	0.064685
77	C	-1.047733	-4.704488	-1.811763
78	C	0.340924	-2.014875	2.049232
79	C	-2.496965	-2.157076	0.069599
80	C	0.484024	-4.415482	2.170572
81	C	1.725898	-2.017890	-0.026397
82	C	-2.376358	-4.700857	0.179794
83	C	-1.190861	-2.162307	-1.884386
84	C	-0.243794	-5.793239	0.165585
85	C	-1.638044	-3.312274	2.142746
86	C	1.050841	-3.319404	-1.886819
87	C	-0.523324	-0.606642	-0.029977
88	U	-0.445268	3.675148	-0.128495
89	C	-1.732276	5.800122	0.490651
90	C	1.711076	3.660943	1.055478
91	C	-1.800770	1.618093	0.567534
92	C	-0.091674	3.624303	-2.562654
93	C	0.545699	1.630433	0.808906
94	C	-1.793544	4.942597	-1.693076
95	C	-0.511935	5.696327	-1.526663
96	C	-0.061576	2.431854	1.916064
97	C	-0.579474	1.604826	-1.452537
98	C	0.613014	5.718903	0.733528
99	C	-0.019679	4.979083	1.869071
100	C	-1.835860	2.394694	-1.646823
101	C	1.599015	2.869899	-1.139534
102	C	-2.182820	3.734564	1.560931
103	C	-2.840982	3.721041	0.239090
104	C	1.623689	4.373608	-1.166795
105	C	0.487253	2.422725	-1.965908
106	C	-2.525093	2.435578	-0.379615
107	C	1.631318	4.848843	0.209023
108	C	-1.447021	4.992830	1.655550
109	C	1.592068	2.445879	0.253166
110	C	0.526401	4.826353	-2.009446
111	C	-1.488620	2.457246	1.702229
112	C	-2.483358	4.971669	-0.425683
113	C	-0.552966	0.922786	-0.046455

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115	C	-1.507615	3.652277	-2.299900
116	C	-0.462313	6.429613	-0.148786
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118	C	-0.718958	-2.129793	-5.351722
119	C	-0.221904	1.883720	-5.344333
120	C	1.292523	-0.334174	-8.367333
121	C	-2.706983	0.160763	-8.028860
122	C	0.863790	1.733435	-7.393979
123	C	-2.127540	-1.929680	-7.191792
124	C	-2.679634	-1.119833	-6.088702
125	C	1.588695	0.898057	-6.417475
126	C	-0.689377	0.656353	-9.073438
127	C	-1.126714	-0.042468	-4.411100
128	C	0.331486	-0.222907	-4.534311
129	C	-0.870790	-0.808027	-9.076449
130	C	-1.635418	2.042621	-7.182619
131	C	1.278046	-1.609698	-6.423595
132	C	0.371542	-2.239033	-7.403233
133	C	-2.369028	1.387864	-6.082803
134	C	-1.841894	1.263198	-8.404384
135	C	0.375231	-1.429263	-8.622965
136	C	-1.475217	1.282920	-4.927014
137	C	0.586336	-1.533177	-5.135664
138	C	-0.280752	2.346829	-6.716876
139	C	-3.035651	0.198738	-6.616223
140	C	1.849427	-0.405877	-7.029573
141	C	-0.888358	-2.556712	-6.728393
142	C	0.670015	0.952319	-8.616586
143	C	0.899974	0.989124	-5.127655
144	C	-2.137570	-1.118337	-8.410644
145	C	-1.786403	-1.238786	-4.935734

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