Electronic Supporting Information

Electronic and photophysical properties of an atomically thin bowl-shaped beryllene encapsulated inside the cavity of [6]Cycloparaphenylene (Be_n@[6]CPP)

Akanksha Ashok Sangolkar, Rama Krishna Kadiyam, Mohmmad Faizan, Omshireesh Chedupaka, Raghasudha Mucherla, and Ravinder Pawar*

Laboratory of Advanced Computation and Theory for Materials and Chemistry, Department of Chemistry, National Institute of Technology Warangal (NITW), Warangal, Telangana-506004, India.

ravinder_pawar@nitw.ac.in

S1: Interaction energy (*IE*) calculated with EDA-ADF and BSSE corrected counterpoise calculation using Gaussian16.

Table S1: Interaction energy (IE_a) between single Be atom and the preceding $Be_{n-1}@[6]CPP$ system.

System	Pauli	Electrostatic	Orbital	IE_a	% Contribution to stabilize the complex		BSSE corrected IE_a
					%Electrostatic	%Orbital	
$Be_1@[6]CPP$	21.86	-11.41	-13.28	-2.83	46.21	53.79	-2.81
$Be_2@[6]CPP$	18.10	-9.75	-12.68	-4.33	43.46	56.54	-4.31
$Be_3@[6]CPP$	28.89	-13.91	-19.28	-4.30	41.90	58.10	-4.28
$Be_4@[6]CPP$	13.33	-7.80	-8.99	-3.46	46.44	53.56	-3.43
$Be_5@[6]CPP$	13.63	-7.78	-11.09	-5.24	41.21	58.79	-5.41
$Be_6@[6]CPP$	25.22	-12.10	-16.91	-3.80	41.70	58.30	-4.02
$Be_7@[6]CPP$	21.42	-9.55	-16.23	-4.35	37.06	62.94	-4.36
$Be_8@[6]CPP$	24.10	-9.07	-19.59	-4.56	31.65	68.35	-4.57
$Be_9@[6]CPP$	24.66	-9.19	-20.88	-5.41	30.57	69.43	-5.39
$Be_{10}@[6]CPP$	21.48	-10.71	-15.02	-4.25	41.61	58.39	-4.25
* All the energy values are given in eV.							

Table S2: Interaction energy (IE_c) to determine the total interaction between Be_n cluster and the distorted [6]CPP in the complex.

System	Pauli	Electrostatic	Orbital	IE_c	% Contribution to stabilize the complex		BSSE corrected IE_c
					%Electrostatic	%Orbital	
Be₁@[6]CPP	21.86	-11.41	-13.28	-2.83	46.21	53.79	-2.81
Be₂@[6]CPP	29.55	-16.23	-18.36	-5.04	46.92	53.08	-5.01
Be₃@[6]CPP	59.97	-30.62	-39.29	-9.94	43.80	56.20	-9.89
Be₄@[6]CPP	60.41	-32.94	-38.09	-10.62	46.37	53.63	-10.56
Be₅@[6]CPP	48.14	-26.81	-31.95	-10.63	45.62	54.38	-9.72
Be₆@[6]CPP	54.95	-28.94	-38.03	-12.02	43.21	56.79	-11.91
Be₇@[6]CPP	43.23	-24.65	-28.35	-9.78	46.51	53.49	-9.70
Be₈@[6]CPP	88.70	-43.59	-59.09	-13.98	42.45	57.55	-13.81
Be₉@[6]CPP	67.18	-37.66	-43.48	-13.96	46.41	53.59	-13.50
Be₁₀@[6]CPP	103.94	-51.51	-71.11	-18.67	42.01	57.99	-18.45

* All the energy values are given in eV.

Table S3: Interaction energy (IE_a) between single Be atom and the preceding Be_{n-1}@[6]CPP system (including dispersion correction).

System	Pauli	Electrostatic	Dispersion	Orbital	IE_a
Be₁@[6]CPP	21.859	-11.411	-0.006	-13.281	-2.838
Be₂@[6]CPP	18.098	-9.748	-0.007	-12.679	-4.335
Be₃@[6]CPP	28.886	-13.907	-0.003	-19.282	-4.306
Be₄@[6]CPP	13.329	-7.797	-0.007	-8.992	-3.467
Be₅@[6]CPP	13.626	-7.777	-0.014	-11.094	-5.258
Be₆@[6]CPP	25.215	-12.098	-0.006	-16.912	-3.802
Be₇@[6]CPP	21.425	-9.553	-0.010	-16.225	-4.364
Be₈@[6]CPP	24.101	-9.072	-0.013	-19.592	-4.576
Be₉@[6]CPP	24.658	-9.190	-0.013	-20.876	-5.421
Be₁₀@[6]CPP	21.478	-10.706	-0.007	-15.020	-4.256

* All the energy values are given in eV.

Table S4: Interaction energy (IE_c) between Be_n cluster and the distorted [6]CPP in the complex (including dispersion correction).

System	Pauli	Electrostatic	Dispersion	Orbital	IE_c
Be₁@[6]CPP	21.859	-11.411	-0.006	-13.281	-2.838
Be₂@[6]CPP	29.552	-16.228	-0.014	-18.362	-5.052
Be₃@[6]CPP	59.970	-30.625	-0.013	-39.288	-9.954
Be₄@[6]CPP	60.411	-32.942	-0.022	-38.094	-10.646
Be₅@[6]CPP	48.137	-26.809	-0.050	-31.954	-10.676
Be₆@[6]CPP	54.948	-28.937	-0.059	-38.030	-12.077
Be₇@[6]CPP	43.225	-24.651	-0.069	-28.351	-9.846
Be₈@[6]CPP	88.695	-43.588	-0.077	-59.086	-14.055
Be₉@[6]CPP	67.177	-37.655	-0.082	-43.482	-14.042
Be₁₀@[6]CPP	103.940	-51.506	-0.090	-71.108	-18.764

* All the energy values are given in eV.

S2: Differential charge density (DCD) plots for Be$_n$@[6]CPP systems

Be$_1$@[6]CPP

Be$_2$@[6]CPP

Be$_3$@[6]CPP

Be$_4$@[6]CPP

Be$_5$@[6]CPP

Be$_6$@[6]CPP

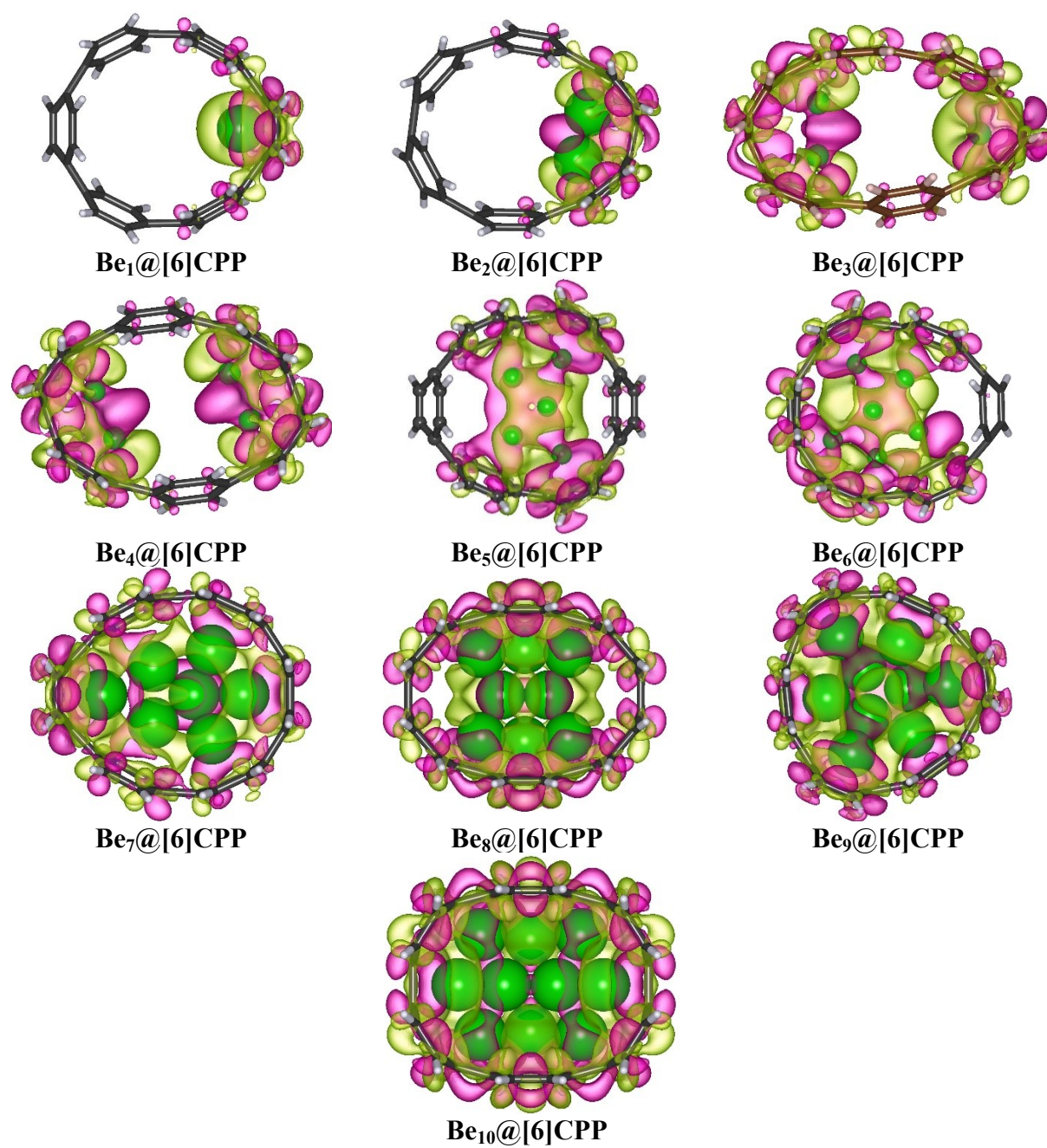**Be$_7$@[6]CPP**

Be$_8$@[6]CPP

Be$_9$@[6]CPP

Be$_{10}$@[6]CPP

Figure S1: The differential charge density (DCD) plots for the Be$_n$@[6]CPP systems

S3: Frontiers molecular orbitals (MOs)

| HOMO | LUMO | HOMO | LUMO |
| Be₁@[6]CPP | | Be₂@[6]CPP | |

HOMO   LUMO   HOMO   LUMO

Be$_1$@[6]CPP   Be$_2$@[6]CPP

HOMO   LUMO   HOMO   LUMO

Be$_3$@[6]CPP   Be$_4$@[6]CPP

HOMO   LUMO   HOMO   LUMO

Be$_5$@[6]CPP   Be$_6$@[6]CPP

HOMO   LUMO   HOMO   LUMO

Be$_7$@[6]CPP   Be$_8$@[6]CPP

HOMO   LUMO   HOMO   LUMO

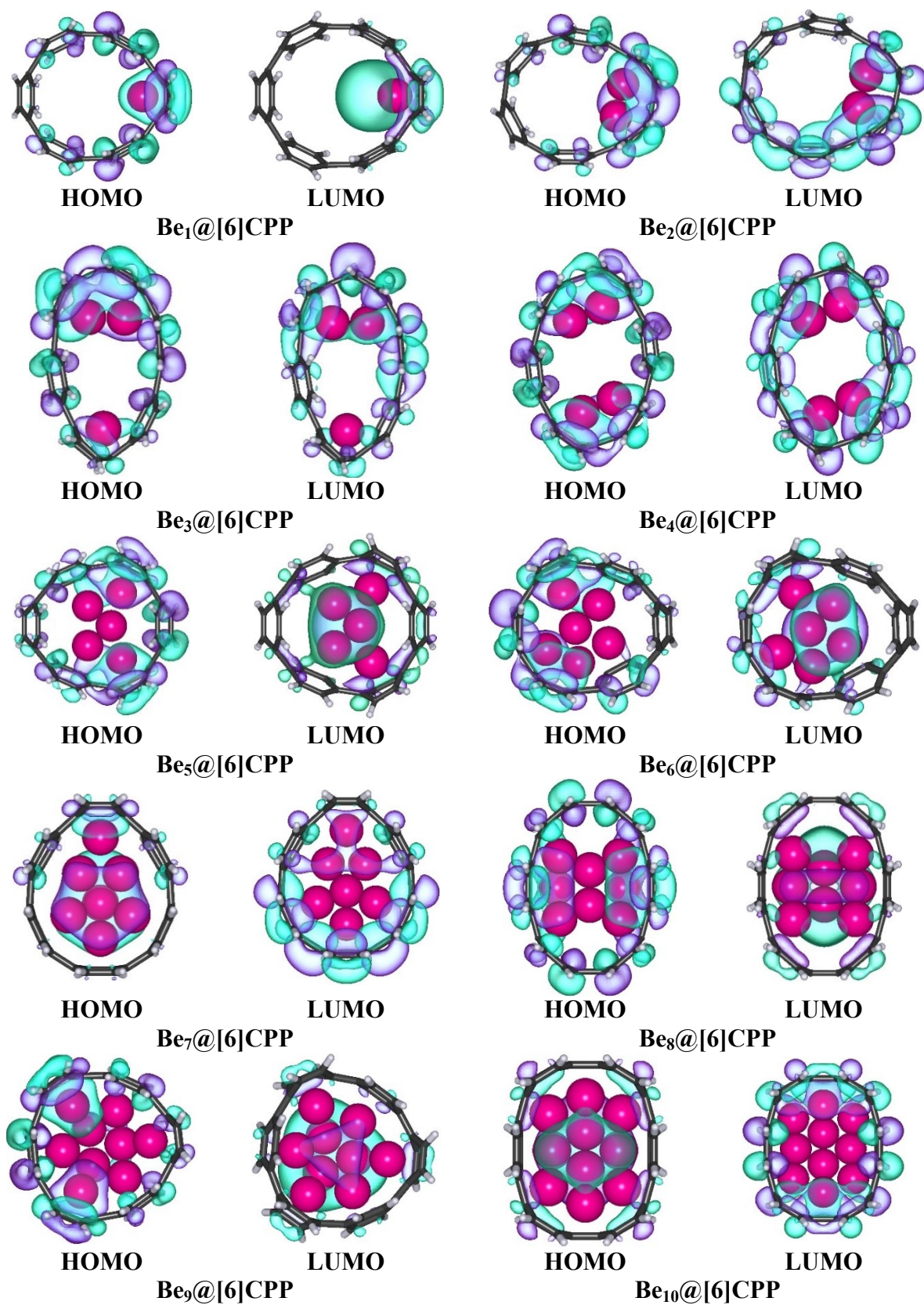Be$_9$@[6]CPP   Be$_{10}$@[6]CPP

Figure S2: The Frontier's Molecular Orbital (MOs) of Be$_n$@[6]CPP systems.
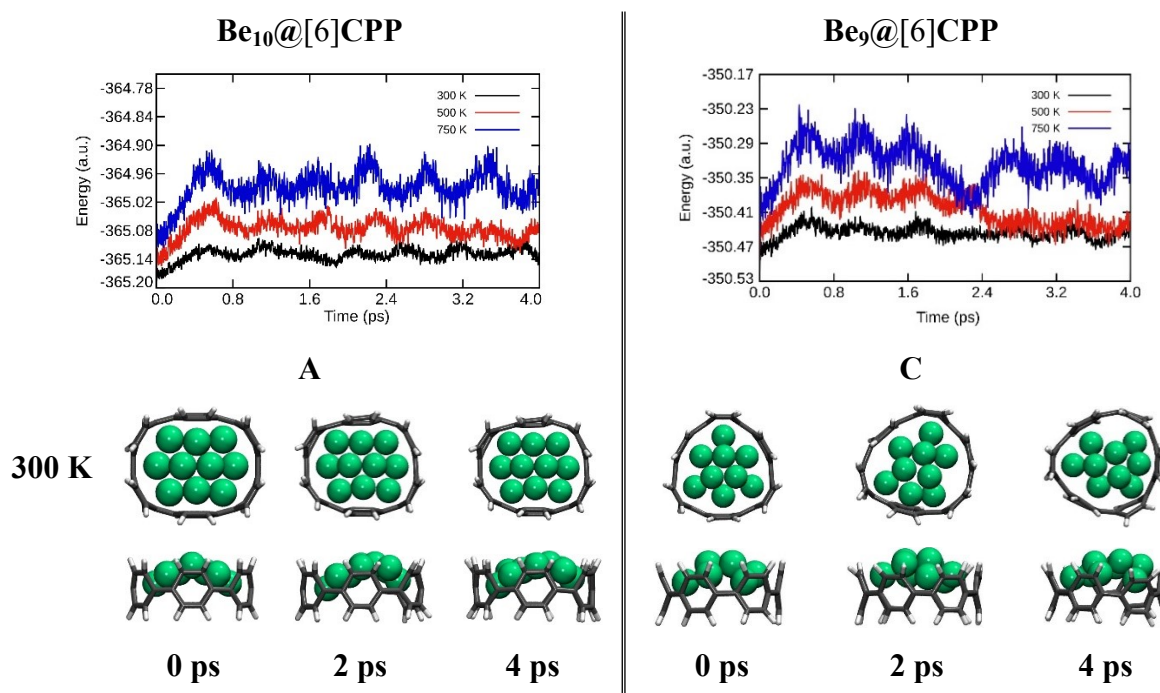
S4: Photophysical properties

Table S5: Spectral Data of the Optical Absorption in Be$_n$@[6]CPP systems.

System	Oscillatory strength	Excitation wavelength (nm)	Molar extinction coefficient (Lmol^{-1}cm^{-1})	Transition	Percentage Contribution
Be1@[6]CPP	0.0048	682.87	166.43	H → L	96.72
	0.2361	349.95	2361.79	H-1 → L+1	63.79
	0.4811	342.45	33297.51	H → L+1	93.95
	0.2190	312.04	34576.49	H-1 → L+2	79.16
	0.2816	303.19	31580.84	H → L+4	67.66
Be2@[6]CPP	0.1061	523.49	4962.57	H → L	85.97
	0.1149	379.46	21259.68	H → L+1	57.66
	0.1829	369.97	23497.48	H-1 → L	59.98
	0.1560	358.81	25093.41	H-1 → L+1	51.71
	0.1922	346.39	25056.14	H-1 → L+1	68.56
	0.1105	326.55	21441.27	H → L+3	86.40
Be3@[6]CPP	0.1097	550.31	4190.99	H → L	95.81
	0.2584	388.50	23675.41	H-1 → L	84.22
	0.1052	357.49	29321.38	H → L+4	48.57
	0.2008	350.72	29293.63	H-1 → L+1	53.97
	0.1658	331.25	25417.39	H-1 → L+2	49.26
Be4@[6]CPP	0.0000	560.91	3726.53	H → L	91.87
	0.2385	427.66	17997.93	H → L+3	54.52
	0.2895	371.43	23220.03	H-2 → L	60.87
	0.1898	350.74	19544.88	H → L+6	49.15
Be5@[6]CPP	0.0117	930.45	508.13	H → L	98.61
	0.0302	545.51	3158.17	H-1 → L	76.47
	0.0320	528.07	3482.22	H → L+3	67.19
	0.1726	383.77	13035.02	H → L+5	62.78
	0.1267	371.41	12069.88	H → L+4	75.49
Be6@[6]CPP	0.0055	1170.4	327.91	H → L	98.32
	0.0371	713.80	2687.18	H → L+1	93.00
	0.1051	513.84	8123.98	H-1 → L+1	74.00
Be7@[6]CPP	0.0021	1163.24	138.52	H → L	98.77
	0.0258	608.95	2911.61	H-1 → L+2	89.57
	0.1205	469.32	5870.04	H → L+4	53.76
Be8@[6]CPP	0.0034	1064.2	578.52	H → L	98.94
	0.0278	669.26	1962.37	H → L+1	97.83
	0.0460	440.82	2617.45	H → L+4	68.94
Be9@[6]CPP	0.0024	1235.86	289.14	H → L	77.12
	0.0216	487.27	5001.12	H-1 → L+3	54.42
	0.1263	473.88	5057.98	H → L+3	45.35
	0.1263	473.88	5057.98	H-1 → L+2	45.15
Be10@[6]CPP	0.0001	1200.56	503.61	H → L	99.18
	0.0474	734.10	2412.31	H → L+2	94.07
	0.2567	468.43	9469.96	H → L+4	61.37

S5: AIMD Simulations

In contrast to the graphene, the atomically thin freestanding layer of metals are thermodynamically unstable. Further, the metals prefer clustering even for the small number of metal atoms due to non-directional nature of the metallic bonding. Despite of this, Rümmeli and co-workers have provided the experimental proofs on the existence of ultrathin metallic structures inside the nanopore of graphene.[1] Likewise, the patches of molybdenum were also achieved by selective removal of selenium atoms from the $MoSe_2$ monolayer.[2] This indicates that the template-assisted growth could be the promising strategy to stabilize an ultrathin metallic nanostructure. However, the atomically thin metal layers are certainly the metastable structures which occupies one of the local minima on the potential energy surface while three-dimensional (3D) clusters locate at the global minimum. Therefore, we cannot expect the stability of these atomically thin metallic framework in a wider temperature range.

AIMD simulations performed at 300K reveals that the $Be_9@[6]CPP$ and $Be_{10}@[6]CPP$ systems are stable at room temperature. Thereafter, attention has been focussed to assess the stability of the studied systems in a wider thermal range and thus the AIMD simulations were performed for $Be_5@[6]CPP$, $Be_9@[6]CPP$ and $Be_{10}@[6]CPP$ systems at 300K, 500K and 750K. The geometry of the systems at different time intervals and the variation in energy during the course of simulations are depicted in Figure S3 and Figure S4.
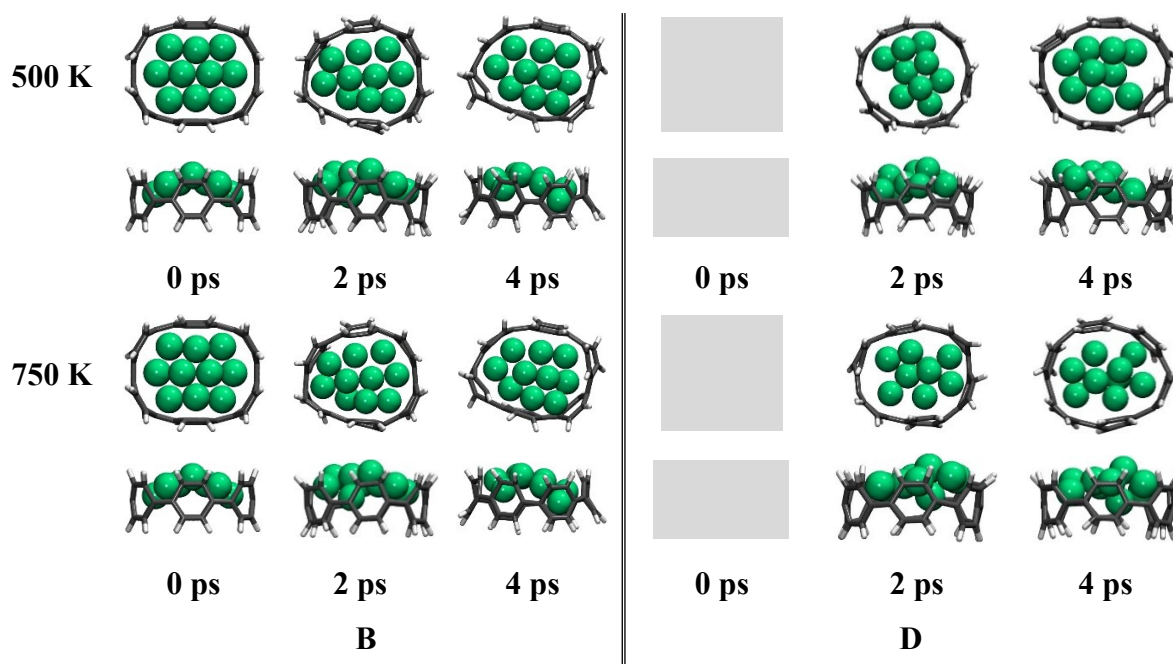
Figure S3. Outcomes of the AIMD simulations. (A) Variation in energy of $Be_{10}@[6]CPP$ at different temperature, (B) Geometry of $Be_{10}@CPP$ system obtained during the simulations, (C) Variation in energy of $Be_9@[6]CPP$ at different temperature, and (D) Geometry of $Be_9@[6]CPP$ system obtained during the simulations.

The ultrathin Be_{10} morphology in $Be_{10}@[6]CPP$ system is maintained with only minor atomic fluctuations during the simulation time of 4 ps at 300K. However, a small space is created inside the $Be_9@[6]CPP$ system even at 300K. Upon increasing the T, the energy of the systems and fluctuation in energy increases. Further, enhanced fluctuation in atomic positions inside the cavity of [6]CPP is observed and the ultrathin structure gets deformed. The distortion is more pronounced in the Be membrane of $Be_9@[6]CPP$ system. Therefore, a significant difference in the energy of the $Be_9@[6]CPP$ system is noticed around 2.4 ps at higher T. It is worth to mention that the systems essentially resist the complete clustering of Be due to strong interactions between the [6]CPP and Be atoms. Interestingly, the AIMD simulations performed for the $Be_5@[6]CPP$ system illustrates the stability of planar Be_5 cluster even at 750K. It has been observed that Be_5 cluster gets tilted inside the cavity of the [6]CPP and regains its position retaining the planarity (Figure S4). Therefore, the AIMD simulations unveils that the [6]CPP can stabilize an ultrathin B_{10} cluster at room temperature and favours slight deformation at higher T range. Noteworthy, the [6]CPP cavity promises to stabilize a few atoms Be cluster (like Be_5) even at 750K with only marginal fluctuations in planarity.
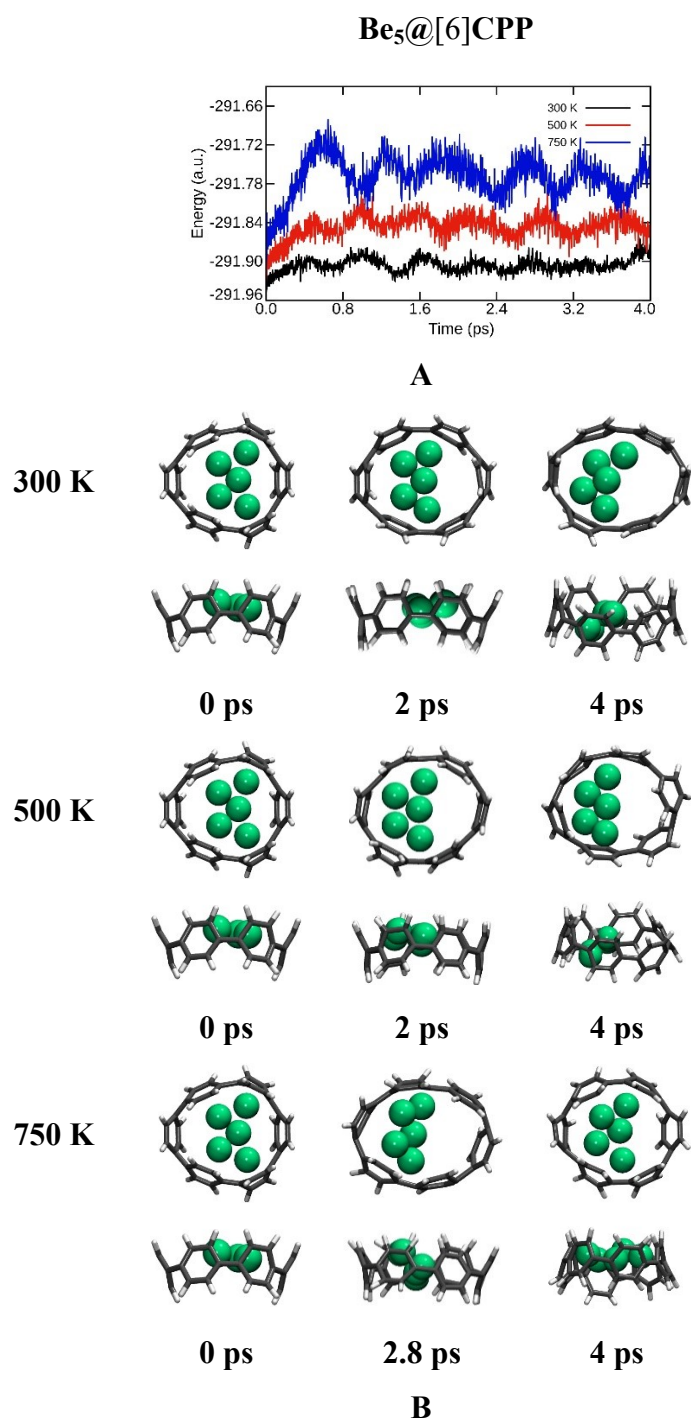
Be$_5$@[6]CPP

A

B

Figure S4. Outcomes of the AIMD simulations. (A) Variation in energy of Be$_5$@[6]CPP at different temperature, (B) Geometry of Be$_5$@[6]CPP system obtained during the simulations.
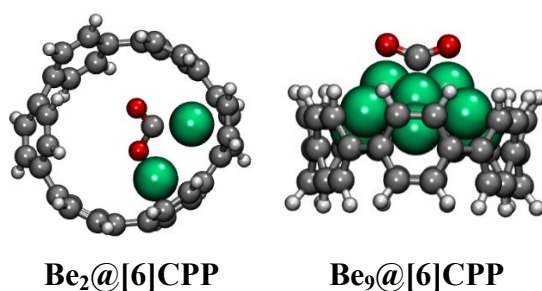
S6: Potential of the systems towards CO_2 activation

Be₂@[6]CPP **Be₉@[6]CPP**

Figure S5. Optimized geometry of CO_2 molecule adsorbed on Be₂@[6]CPP and Be₉@[6]CPP systems.

S7: 2D vs 3D stability

3D Be₅ **Planar Be₅**

Figure S6. Top and side view of the optimized geometry of 3D and planar Be₅ cluster inside the cavity of [6]CPP.

The most stable 3D Be₅ cluster reported in a recent work was considered as an initial guess inside the [6]CPP cavity during geometry optimization.[3] The free energy (ΔG) difference between the encapsulated systems with planar and 3D Be₅ arrangement calculated with the M062X/6-311+G** level of theory is found to be -13.16 kcal/mol. Therefore, it is worth to mention that the planar Be₅ cluster is favoured over the 3D cluster inside the [6]CPP cavity. This indicates that the 3D cluster occupies minima lower than the 3D cluster in the gas phase. In contrast to this, the system with planar Be₅ cavity occupies minima lower than the 3D cluster when encapsulated inside the [6]CPP cavity. This may be attributed to the stronger electrostatic and orbital interaction of the Be atoms with the [6]CPP architecture. The size of the planar Be₅ cluster achieved inside the [6]CPP resembles the other metal patches experimentally observed inside a nanopore of graphene. This suggests that the [6]CPP could serve as a promising template to stabilize a few Be atoms cluster in an atomically thin arrangement.

Cartesian Coordinates of optimized Be$_n$@[6]CPP systems

1. **Be$_1$@[6]CPP**

C	-0.84129600	-3.92389200	-0.15441100
C	-1.68766300	-4.08441900	0.95511100
C	-2.92603700	-3.45793600	1.00490900
C	-3.36913400	-2.65633800	-0.05813300
C	-2.66339400	-2.76731200	-1.26199700
C	-1.42462000	-3.38814800	-1.30883600
H	-1.32931600	-4.60379300	1.83691700
H	-3.49771400	-3.49579200	1.92607400
H	-2.98397200	-2.19702700	-2.12562600
H	-0.83600200	-3.28006800	-2.21156600
C	0.64103900	-3.89257900	-0.03527300
C	1.47848400	-3.81386700	-1.15827700
C	1.20764200	-3.50938200	1.18836200
C	2.69071300	-3.13833200	-1.10642600
H	1.13830900	-4.19792800	-2.11384800
C	2.42653500	-2.85220900	1.25088400
H	0.62328300	-3.58593300	2.09774400
C	3.11615900	-2.50713000	0.07809600
H	3.25132700	-3.00366100	-2.02572500
H	2.75448100	-2.44346900	2.19990400
C	3.96733200	-1.29765500	0.08403000
C	4.51389900	-0.67124400	1.32708400
C	4.56522500	-0.70508700	-1.14051700
C	4.51443200	0.66917000	1.32710200
H	4.97321800	-1.27366600	2.10594400
C	4.56577300	0.70302900	-1.14050200
H	4.87053300	-1.27206900	-2.01272600
C	3.96837200	1.29602300	0.08405800
H	4.97423700	1.27119800	2.10597700
H	4.87144500	1.26976900	-2.01274200
C	-4.15556400	-1.40875400	0.14253600
C	-4.71874200	-0.69280800	-0.92640900
C	-3.91827100	-0.69299700	1.32124500
C	-4.71836400	0.69503000	-0.92640300
H	-5.03519900	-1.21944200	-1.82038800
C	-3.91789200	0.69476600	1.32125100
H	-3.52139200	-1.20512700	2.18966400
C	-4.15479400	1.41066100	0.14254700
H	-5.03453300	1.22184400	-1.82037800
H	-3.52073100	1.20667300	2.18967200

C	-0.83923600	3.92415100	-0.15442000
C	-1.68551500	4.08508300	0.95511200
C	-1.42282300	3.38865800	-1.30883000
C	-2.92419100	3.45919800	1.00492500
H	-1.32691300	4.60429400	1.83691000
C	-2.66189800	2.76842600	-1.26197700
H	-0.83426700	3.28028600	-2.21156500
C	-3.36769700	2.65782300	-0.05811500
H	-3.49584300	3.49733800	1.92609400
H	-2.98276000	2.19828900	-2.12559800
C	0.64308500	3.89222600	-0.03531400
C	1.48046400	3.81310300	-1.15833500
C	1.20958900	3.50890700	1.18833400
C	2.69244000	3.13711400	-1.10647700
H	1.14041700	4.19723500	-2.11392400
C	2.42823500	2.85128500	1.25087700
H	0.62529800	3.58577300	2.09773400
C	3.11768300	2.50582500	0.07808600
H	3.25299300	3.00218500	-2.02577500
H	2.75607400	2.44251700	2.19992000
Be	3.04680700	-0.00043300	-0.62901900

2. Be$_2$@[6]CPP

C	-3.29412300	-2.76343000	0.14905300
C	-3.47673500	-2.02463600	1.32337500
C	-4.12827100	-0.80125600	1.29671400
C	-4.61357900	-0.27487100	0.09343300
C	-4.74387300	-1.17630200	-0.97599400
C	-4.09167800	-2.40104200	-0.94900200
H	-2.92530500	-2.28671900	2.21803200
H	-4.05042600	-0.16452000	2.16941900
H	-5.23103700	-0.86096600	-1.89236000
H	-4.09231400	-3.01498400	-1.84319100
C	-2.00653200	-3.49084000	-0.00570100
C	-1.31482100	-3.33593100	-1.21519800
C	-1.25434400	-3.93264200	1.09070500
C	0.06873800	-3.35913700	-1.25888900
H	-1.84958700	-3.02288400	-2.10360400
C	0.13439500	-3.94462000	1.05102600
H	-1.75046700	-4.16577000	2.02638600
C	0.82920300	-3.52324400	-0.09158900
H	0.55040600	-3.07724400	-2.18997300
H	0.67441400	-4.19631500	1.95588500
C	2.21046900	-2.98412800	-0.03337100
C	2.86287400	-2.63542500	1.22046200
C	3.03347400	-2.81980900	-1.18185000

C	3.94209300	-1.81536000	1.26652400
H	2.45131200	-3.02012900	2.14598100
C	4.03590700	-1.84652100	-1.17924900
H	2.77102700	-3.30136600	-2.11782700
C	4.29825100	-1.08955400	0.05118500
H	4.40622000	-1.56555000	2.21131700
H	4.58526300	-1.63174000	-2.08541700
C	-4.42271800	1.18741100	-0.11289900
C	-3.78779100	1.56821300	-1.30150800
C	-4.34370500	2.09226200	0.95818400
C	-2.85588500	2.59501500	-1.31225000
H	-3.84842800	0.92678800	-2.17229700
C	-3.40959700	3.11854800	0.94776000
H	-4.91342200	1.90972100	1.86307500
C	-2.52703900	3.27394000	-0.13395100
H	-2.23544800	2.71304900	-2.19248500
H	-3.27648200	3.71817700	1.84174900
C	1.68176400	3.23651200	0.14536200
C	0.88592000	3.14860500	1.29611200
C	1.08185300	3.80680000	-0.99033500
C	-0.47993000	3.37213800	1.24050900
H	1.30431600	2.74185300	2.20919400
C	-0.28666300	4.03382700	-1.04203200
H	1.66771700	3.98919800	-1.88419700
C	-1.11711700	3.70881000	0.03925600
H	-1.07674800	3.12488200	2.11053700
H	-0.72459700	4.38183600	-1.97146600
C	2.96164700	2.49754400	0.10110500
C	3.68961900	2.24266400	-1.10702200
C	3.68190900	2.10881200	1.32458900
C	4.48328000	1.09686200	-1.17100800
H	3.48333000	2.79000100	-2.02018700
C	4.53985700	1.07260800	1.30109500
H	3.54889100	2.70890900	2.21945200
C	4.56237600	0.27846200	0.05601700
H	4.97351800	0.81494100	-2.09360800
H	5.15665600	0.81266700	2.15316700
Be	2.21193400	-1.16947000	-0.80826500
Be	2.64452200	0.75808000	-0.66706000

3. Be$_3$@[6]CPP

C	-2.43821700	2.75729900	0.10635800
C	-1.59640000	2.88480800	1.25706600
C	-0.23287400	2.97171400	1.14797600
C	0.44733100	2.98095900	-0.10182200

C	-0.35970800	3.02743900	-1.22252200
C	-1.75695600	2.86659700	-1.14995500
H	-2.04322400	2.82333400	2.24152500
H	0.34086300	2.97163100	2.06688300
H	0.07522700	3.10420600	-2.21173100
H	-2.32465800	2.91937900	-2.07225900
C	-3.71913600	2.09518300	0.16330200
C	-4.43837200	1.74453500	-1.06277300
C	-4.32274200	1.55904300	1.38219000
C	-5.12917100	0.57208900	-1.11398300
H	-4.41765500	2.40346000	-1.92502600
C	-5.02761200	0.41125600	1.32586800
H	-4.19411800	2.07909500	2.32566900
C	-5.01883400	-0.30513500	0.04041000
H	-5.63264500	0.26090600	-2.02243600
H	-5.47873700	-0.01943400	2.21136600
C	-4.43415200	-1.55264400	-0.05246200
C	-4.02301400	-2.30484400	1.14583800
C	-3.88620200	-2.10999500	-1.30497600
C	-2.77084800	-2.80055100	1.17015400
H	-4.68343000	-2.37832600	2.00067000
C	-2.64422200	-2.74628400	-1.24950600
H	-4.39246400	-1.97362800	-2.25123000
C	-1.92059800	-2.75339700	-0.01946100
H	-2.37804600	-3.27168500	2.06534200
H	-2.15972500	-3.01778700	-2.18102500
C	1.90087200	2.70462600	-0.18176200
C	2.48398800	2.23228800	-1.33182200
C	2.74308600	2.74108500	0.98104000
C	3.75247800	1.58136100	-1.35542700
H	1.94625000	2.25997900	-2.27231800
C	3.96242500	2.14174500	1.03384400
H	2.39556300	3.25805000	1.86844300
C	4.48254200	1.39366700	-0.08973900
H	4.26299500	1.47204300	-2.30582900
H	4.55021700	2.17851000	1.94225900
C	3.69387900	-1.74480900	0.15264200
C	4.42721300	-1.43775800	1.41354400
C	4.56676500	-1.74678600	-1.01649200
C	5.33877300	-0.45614800	1.37636200
H	4.28039300	-2.07921800	2.27873600
C	5.44823300	-0.66817400	-1.09529500
H	4.43393700	-2.42940200	-1.84993200
C	5.32144400	0.26562800	0.06647500
H	6.05020200	-0.25485500	2.16837100
H	6.06470200	-0.48616300	-1.96767700

C	2.35596900	-2.38549400	0.17089000
C	1.74746500	-2.94122700	-0.96225900
C	1.54740400	-2.22453900	1.30377100
C	0.37959800	-3.18756300	-1.00489700
H	2.32970600	-3.12710000	-1.85853300
C	0.18477200	-2.46188500	1.25862600
H	1.97273600	-1.79829800	2.20548000
C	-0.44934300	-2.88052900	0.08072600
H	-0.04717800	-3.56816200	-1.92639700
H	-0.41342500	-2.20568800	2.12559200
Be	-2.41996400	-0.98895800	-0.67105100
Be	-2.38518600	1.01908400	-0.63274200
Be	3.74702400	-0.14567300	-0.75308700

4. **Be₄@[6]CPP**

C	2.13558900	-2.98147000	0.13620300
C	1.40659300	-2.86247000	1.32896100
C	0.03242700	-3.02495900	1.35276800
C	-0.68808200	-3.33607400	0.19167700
C	0.06736300	-3.68614600	-0.93584200
C	1.44520800	-3.51314900	-0.96386200
H	1.89704900	-2.48370000	2.21840200
H	-0.49101600	-2.76874800	2.26560300
H	-0.42361200	-4.01190500	-1.84631900
H	1.96703900	-3.70620300	-1.89433700
C	3.42611900	-2.27435900	0.01523600
C	4.05176200	-1.98588500	-1.24690800
C	4.23538900	-1.89526200	1.18791000
C	4.77766700	-0.79972200	-1.35287600
H	3.81221600	-2.54195700	-2.14683100
C	5.02772200	-0.81247100	1.11504900
H	4.22515900	-2.53908800	2.06303100
C	4.86456500	0.00419800	-0.11249300
H	5.19952400	-0.48297400	-2.29822900
H	5.73200600	-0.54519300	1.89442000
C	4.41325400	1.32201600	-0.05367100
C	4.08964800	1.97575300	1.20819600
C	3.96726700	2.08731600	-1.22495700
C	2.92896100	2.67345700	1.28075500
H	4.67004500	1.76888500	2.09743600
C	2.87331600	2.95341200	-1.10723400
H	4.45597200	1.95810700	-2.18084500
C	2.12965500	2.97966700	0.10580600
H	2.58087100	3.02250600	2.24610900
H	2.48235800	3.41254800	-2.00866900

C	-2.12965600	-2.97966500	0.10571600
C	-2.87329800	-2.95339000	-1.10733500
C	-2.92898100	-2.67347400	1.28065800
C	-3.96724600	-2.08729100	-1.22506100
H	-2.48232800	-3.41251300	-2.00877200
C	-4.08966600	-1.97576800	1.20809100
H	-2.58090600	-3.02253800	2.24601200
C	-4.41325100	-1.32201000	-0.05377000
H	-4.45593600	-1.95806600	-2.18095500
H	-4.67007700	-1.76891400	2.09732500
C	-3.42611900	2.27435500	0.01521700
C	-4.23541400	1.89524400	1.18786800
C	-4.05173700	1.98590500	-1.24694500
C	-5.02774900	0.81245600	1.11497400
H	-4.22520000	2.53905700	2.06299900
C	-4.77764600	0.79974800	-1.35294700
H	-3.81217200	2.54199200	-2.14685400
C	-4.86456700	-0.00419300	-0.11257800
H	-5.73205200	0.54516800	1.89432500
H	-5.19948600	0.48301600	-2.29831300
C	-2.13559000	2.98146200	0.13622100
C	-1.44519200	3.51317000	-0.96381900
C	-1.40661400	2.86242900	1.32898700
C	-0.06734800	3.68617000	-0.93577200
H	-1.96700900	3.70624800	-1.89429700
C	-0.03244800	3.02492000	1.35282100
H	-1.89708300	2.48363400	2.21840900
C	0.68807900	3.33606900	0.19175000
H	0.42364200	4.01195400	-1.84623200
H	0.49098100	2.76868400	2.26565700
Be	2.99158200	-0.56061600	-0.68307400
Be	2.20183700	1.24202100	-0.80585500
Be	-2.99158100	0.56061800	-0.68311000
Be	-2.20180500	-1.24200600	-0.80592100

5. <u>Be₅@[6]CPP</u>

C	3.86766700	1.40243400	0.38327200
C	3.63038300	0.69318200	1.57048400
C	3.63036700	-0.69330100	1.57048600
C	3.86763200	-1.40256100	0.38327400
C	4.48355500	-0.69406800	-0.65588600
C	4.48357300	0.69392300	-0.65588700
H	3.23072300	1.21689600	2.43302300
H	3.23069200	-1.21700400	2.43302500
H	4.82448900	-1.21256200	-1.54498500

H	4.82452100	1.21240700	-1.54498600
C	3.09063300	2.63554100	0.12046100
C	2.79067300	3.05096900	-1.21292400
C	2.67503600	3.58554400	1.17352700
C	1.55587100	3.67804900	-1.41729800
H	3.36853200	2.72067900	-2.06832600
C	1.53380800	4.26956500	0.99803900
H	3.34331900	3.76693000	2.01052800
C	0.74766800	3.87685400	-0.19741600
H	1.22514200	3.98745600	-2.40179600
H	1.23053400	5.08193100	1.65025300
C	-0.64607800	3.66722600	-0.21525200
C	-1.47023600	3.89168200	0.93453400
C	-1.30444700	3.04467400	-1.35490200
C	-2.70973500	3.32768000	1.05298500
H	-1.06733100	4.47204900	1.75545900
C	-2.60396400	2.48985200	-1.18901300
H	-0.91116400	3.18060800	-2.35627700
C	-3.27319400	2.51173000	0.03031800
H	-3.26574200	3.46700000	1.97449400
H	-3.03991500	1.95757900	-2.02793000
C	3.09055800	-2.63564400	0.12046300
C	2.79058200	-3.05106500	-1.21292000
C	2.67491600	-3.58562300	1.17353300
C	1.55575100	-3.67808900	-1.41729300
H	3.36845300	-2.72079900	-2.06832300
C	1.53365800	-4.26959400	0.99804500
H	3.34318700	-3.76703300	2.01053700
C	0.74753700	-3.87685800	-0.19741300
H	1.22500800	-3.98748300	-2.40179100
H	1.23034600	-5.08194100	1.65026500
C	-3.27329500	-2.51164100	0.03030700
C	-2.70985600	-3.32760400	1.05297700
C	-2.60406500	-2.48977900	-1.18902100
C	-1.47036800	-3.89162800	0.93453100
H	-3.26587000	-3.46691500	1.97448300
C	-1.30455400	-3.04462500	-1.35490700
H	-3.03999800	-1.95748900	-2.02793600
C	-0.64620300	-3.66719100	-0.21525400
H	-1.06747900	-4.47200500	1.75545600
H	-0.91127900	-3.18058300	-2.35628200
C	-4.18837700	-1.38951200	0.32200300
C	-4.83701700	-0.69212600	-0.71026500
C	-3.96367900	-0.69333200	1.51476500
C	-4.83698600	0.69227900	-0.71026300
H	-5.18022100	-1.22477200	-1.59099000

C	-3.96364900	0.69344000	1.51476700
H	-3.53892400	-1.20557500	2.37043100
C	-4.18831700	1.38963400	0.32200800
H	-5.18016800	1.22494300	-1.59098500
H	-3.53887200	1.20566200	2.37043600
Be	1.33279500	2.06966200	-0.56951400
Be	-0.80136600	1.25361900	-0.90967800
Be	-0.80138600	-1.25360700	-0.90968800
Be	1.33275400	-2.06968300	-0.56952100
Be	0.69393300	-0.00000700	-0.58584100

6. $\underline{Be_6@[6]CPP}$

C	-3.95783400	-1.50766000	0.34549500
C	-4.04436600	-0.70407300	1.54278200
C	-4.01594400	0.65326500	1.44823800
C	-3.98239500	1.33304700	0.18244500
C	-4.34067000	0.59114100	-0.91656900
C	-4.28741200	-0.83210500	-0.89150300
H	-4.00496400	-1.18472600	2.51311900
H	-3.92795200	1.23700100	2.35879000
H	-4.44672900	1.05598900	-1.89000200
H	-4.63447200	-1.39574400	-1.74888400
C	-3.17113400	-2.69653300	0.26663500
C	-2.76596700	-3.20394000	-1.06192800
C	-2.56348700	-3.37379300	1.41623300
C	-1.47113000	-3.77499000	-1.14299900
H	-3.45924000	-3.33198500	-1.88688500
C	-1.32464700	-3.87627300	1.29128700
H	-3.11302200	-3.45490100	2.34803600
C	-0.63863400	-3.80401100	-0.00145800
H	-1.10338500	-4.11751500	-2.10689600
H	-0.81672700	-4.34615300	2.12584700
C	0.82557600	-3.66991000	-0.14915400
C	1.73884600	-3.96524300	0.80406800
C	1.19661300	-2.78763700	-1.32407300
C	3.06431100	-3.37105500	0.83026800
H	1.44092600	-4.56711200	1.65656700
C	2.52790700	-2.07089100	-1.20326300
H	1.02579300	-3.25819700	-2.29582500
C	3.41488400	-2.41546800	-0.05799100
H	3.69478700	-3.56869600	1.69022600
H	3.05685000	-1.95859200	-2.14878000
C	-3.17076100	2.56332400	0.04359000
C	-2.80793500	3.08294100	-1.23859600
C	-2.79463500	3.43343500	1.18006700

C	-1.55489300	3.69695300	-1.33687300
H	-3.35933700	2.85128600	-2.14261800
C	-1.63038200	4.09729300	1.11069400
H	-3.49740300	3.57909500	1.99516100
C	-0.79842700	3.78767700	-0.07605100
H	-1.17649900	4.07796200	-2.27830300
H	-1.33947700	4.84719400	1.83875100
C	3.28325900	2.56594000	0.11748700
C	2.67038600	3.27677900	1.19194400
C	2.62727300	2.60510500	-1.10282300
C	1.40288800	3.78188600	1.10525000
H	3.20977500	3.37492500	2.12827000
C	1.30271000	3.11319300	-1.24527800
H	3.07941300	2.13461200	-1.96883300
C	0.60678900	3.62042100	-0.07306800
H	0.96304800	4.27218500	1.96520500
H	0.92224900	3.32207300	-2.23925100
C	4.25199700	1.47065500	0.34438900
C	4.89230400	0.83829100	-0.73386400
C	4.08982400	0.72040600	1.51473600
C	4.92858100	-0.54458900	-0.79439400
H	5.17635500	1.41356400	-1.60870700
C	4.14877000	-0.66512400	1.45903800
H	3.66712000	1.17759200	2.40184700
C	4.36085100	-1.30999400	0.23608400
H	5.22833100	-1.02400200	-1.72032900
H	3.76678300	-1.23308400	2.29950500
Be	-0.51768300	-2.09145500	-0.92472300
Be	1.28594900	-0.91642200	-1.03637400
Be	0.69185200	1.36975600	-0.90430200
Be	-1.41401700	2.01403600	-0.61279700
Be	-0.69835200	-0.03063400	-0.74792200
Be	-2.45547900	-1.30866800	-0.71665400

7. Be₇@[6]CPP

C	0.75239400	3.84932300	0.16072600
C	1.47294100	3.75537000	1.34843800
C	2.74589100	3.16816400	1.37673300
C	3.35124400	2.66591200	0.23125400
C	2.77002700	3.05498600	-1.01544700
C	1.49127100	3.64288100	-1.04652300
H	0.98531700	3.94384200	2.29644600
H	3.16821500	2.94462000	2.34928600
H	3.33247900	2.96632700	-1.93441000
H	1.10314600	3.99368200	-1.99490100

C	-0.70759500	3.76203500	0.10675100
C	-1.28083700	3.28484700	-1.10651000
C	-1.50972000	3.67719800	1.24747400
C	-2.48283700	2.58009100	-1.11038500
H	-0.83522900	3.51758200	-2.06262700
C	-2.73345400	3.01984100	1.25884500
H	-1.13863900	4.06996200	2.18789400
C	-3.20407000	2.34320800	0.11868000
H	-2.93864300	2.32530300	-2.06165100
H	-3.27453100	2.92169600	2.19156200
C	-4.16771900	1.29063900	0.15000700
C	-4.71408900	0.66983600	1.38541600
C	-4.65602100	0.68918600	-1.09970700
C	-4.71406400	-0.66988800	1.38540900
H	-5.14445300	1.26601300	2.18465100
C	-4.65599800	-0.68921700	-1.09971000
H	-4.92374100	1.27059500	-1.97683600
C	-4.16767300	-1.29066300	0.14999500
H	-5.14440100	-1.26609000	2.18464000
H	-4.92369400	-1.27062800	-1.97684600
C	4.14704200	1.42506100	0.23715500
C	4.24567700	0.71180200	-1.01746400
C	4.37883400	0.70993500	1.39049000
C	4.24567600	-0.71175900	-1.01746800
H	4.51919700	1.24381400	-1.92007100
C	4.37884200	-0.70988800	1.39048800
H	4.33400500	1.20144200	2.35478700
C	4.14705300	-1.42501600	0.23715600
H	4.51921600	-1.24377100	-1.92006900
H	4.33402000	-1.20139700	2.35478500
C	0.75244100	-3.84932000	0.16073900
C	1.47298500	-3.75535200	1.34844800
C	1.49130600	-3.64286800	-1.04651500
C	2.74592800	-3.16812600	1.37673900
H	0.98536800	-3.94382600	2.29645800
C	2.77005900	-3.05496700	-1.01544500
H	1.10318400	-3.99369700	-1.99488600
C	3.35126900	-2.66587300	0.23125800
H	3.16824600	-2.94456400	2.34929000
H	3.33253200	-2.96634200	-1.93439900
C	-0.70754900	-3.76205500	0.10675900
C	-1.28078100	-3.28487600	-1.10650500
C	-1.50968500	-3.67722700	1.24747500
C	-2.48278000	-2.58012200	-1.11039000
H	-0.83514100	-3.51758400	-2.06261500
C	-2.73342400	-3.01987800	1.25883100

H	-1.13861200	-4.06998800	2.18789900
C	-3.20402700	-2.34324200	0.11866400
H	-2.93855500	-2.32529900	-2.06166000
H	-3.27451100	-2.92173700	2.19154300
Be	-2.98010500	0.00001300	-0.57036900
Be	-0.99429800	-1.09454800	-1.18557600
Be	1.27281000	-1.72107800	-1.28230200
Be	0.59548900	0.00000900	-1.74982800
Be	2.53618800	0.00003300	-1.39900000
Be	-0.99433800	1.09451900	-1.18559000
Be	1.27272800	1.72109500	-1.28219300

8. Be$_8$@[6]CPP

C	2.81798900	-2.86549600	0.22005500
C	3.43697700	-2.50832000	-1.04517500
C	4.37751900	-1.43984600	-1.06268600
C	4.69364500	-0.74198500	0.08217400
C	4.43720800	-1.43489000	1.31972600
C	3.55419900	-2.46197200	1.39855000
H	3.27557300	-3.10805900	-1.93211000
H	4.65903700	-1.05901800	-2.03803600
H	4.90066700	-1.08197700	2.23388900
H	3.33844300	-2.92505600	2.35368700
C	1.44393000	-3.22916700	0.22688800
C	0.67333000	-3.44302100	1.43976300
C	0.74571700	-3.33889600	-1.08688900
C	-0.67313400	-3.44257300	1.43982200
H	1.20603800	-3.57846300	2.37319400
C	-0.74557400	-3.33851900	-1.08671700
H	1.19196400	-3.99600400	-1.83201900
C	-1.44362400	-3.22841400	0.22690700
H	-1.20589300	-3.57762100	2.37327400
H	-1.19241700	-3.99509500	-1.83194800
C	-2.81766900	-2.86456800	0.21998400
C	-3.43663900	-2.50750200	-1.04523900
C	-3.55400700	-2.46132300	1.39847500
C	-4.37786500	-1.43969400	-1.06278700
H	-3.27475800	-3.10700900	-1.93224000
C	-4.43758200	-1.43474300	1.31966000
H	-3.33799500	-2.92429200	2.35360700
C	-4.69429600	-0.74197200	0.08208500
H	-4.65956500	-1.05898900	-2.03813100
H	-4.90122600	-1.08203500	2.23380500
C	4.69364000	0.74198000	0.08217400
C	4.43719900	1.43488200	1.31972500

C	4.37751100	1.43983900	-1.06268600
C	3.55418900	2.46196500	1.39854900
H	4.90065000	1.08196500	2.23389000
C	3.43696500	2.50830800	-1.04517400
H	4.65902500	1.05900800	-2.03803600
C	2.81798400	2.86549400	0.22005300
H	3.33842600	2.92504200	2.35368700
H	3.27554700	3.10803400	-1.93211500
C	-1.44362500	3.22842500	0.22690600
C	-0.74557400	3.33852800	-1.08671800
C	-0.67313700	3.44260300	1.43981800
C	0.74571200	3.33890600	-1.08689000
H	-1.19242100	3.99509500	-1.83195600
C	0.67332700	3.44305200	1.43976000
H	-1.20589600	3.57767000	2.37326800
C	1.44392600	3.22917800	0.22688700
H	1.19196300	3.99600500	-1.83202600
H	1.20603500	3.57851300	2.37318800
C	-2.81766900	2.86456500	0.21998200
C	-3.55400000	2.46131100	1.39847400
C	-3.43663200	2.50748700	-1.04523800
C	-4.43757400	1.43473000	1.31966000
H	-3.33798100	2.92427300	2.35360800
C	-4.37786100	1.43968200	-1.06278700
H	-3.27473700	3.10698000	-1.93224500
C	-4.69429200	0.74196100	0.08208500
H	-4.90121000	1.08201700	2.23380700
H	-4.65955600	1.05897500	-2.03813100
Be	-1.75999600	-1.68375000	-0.75769300
Be	1.76059100	-1.68506700	-0.75810600
Be	-1.75997200	1.68374800	-0.75766400
Be	1.76056500	1.68506600	-0.75807700
Be	0.00027900	-1.84161300	-1.80535100
Be	-0.97849000	0.00000700	-1.73703000
Be	0.00027900	1.84162100	-1.80536200
Be	0.97649400	0.00000600	-1.73296100

9. <u>Be$_9$@[6]CPP</u>

C	-3.56776300	-1.84039900	0.17231100
C	-3.72434500	-1.09809400	1.37772800
C	-3.86157800	0.26720500	1.37616800
C	-3.86363600	1.02514100	0.17072300
C	-4.07730000	0.27311600	-1.00814400
C	-3.93185900	-1.14766300	-1.00878800
H	-3.59015300	-1.60849400	2.32391700

H	-3.83312000	0.79497400	2.32204300
H	-4.28385300	0.77507600	-1.94689300
H	-4.03576400	-1.68229400	-1.94647700
C	-2.79585400	-3.07162200	0.17635800
C	-2.45458800	-3.82051400	-1.03214100
C	-2.39404900	-3.75887500	1.43261200
C	-1.17003600	-4.37548200	-1.03110000
H	-3.08061500	-3.86058600	-1.91710400
C	-1.16519100	-4.28720100	1.43180700
H	-3.10335900	-3.91490300	2.24068700
C	-0.39010500	-4.11156400	0.17492900
H	-0.76849900	-4.85541500	-1.91729900
H	-0.78963700	-4.90804200	2.24059500
C	1.04357600	-3.85741400	0.17119300
C	1.69911600	-3.47590100	1.37637900
C	1.80177000	-3.66730800	-1.00777200
C	2.81310700	-2.67474000	1.37733800
H	1.22746400	-3.71409900	2.32234000
C	2.95979300	-2.83135100	-1.00908100
H	1.47024500	-4.09744600	-1.94636600
C	3.37800300	-2.16903600	0.17158400
H	3.18794000	-2.30264800	2.32328800
H	3.47447900	-2.65428600	-1.94696900
C	-3.36677800	2.39362600	0.17441700
C	-3.20455800	3.20107700	-1.03150800
C	-3.13148100	3.15254300	1.43157000
C	-2.08143100	4.03583200	-1.03192600
H	-3.82062600	3.09345300	-1.91797100
C	-2.05920700	3.95210300	1.43273600
H	-3.85747000	3.13805200	2.23985400
C	-1.26268100	3.95623300	0.17682600
H	-1.80268800	4.59838700	-1.91651400
H	-1.83989600	4.64462700	2.24068200
C	2.81955800	2.83247300	0.17123400
C	2.16153800	3.20808800	1.37685100
C	2.27527200	3.39476500	-1.00718100
C	0.91055900	3.77198900	1.37862400
H	2.60376300	2.91768200	2.32242000
C	0.97197500	3.97895700	-1.00757500
H	2.81342700	3.32383000	-1.94593900
C	0.18971400	4.00870600	0.17330100
H	0.40135300	3.91042300	2.32485600
H	0.56087000	4.33694000	-1.94496900
C	3.75678000	1.71831400	0.17418000
C	4.37501500	1.17493300	-1.03220500
C	4.29682800	1.13470400	1.43084000

C	4.53646400	-0.21510800	-1.03337200
H	4.58985400	1.76271100	-1.91837400
C	4.45370600	-0.19369500	1.43130200
H	4.64690300	1.77036900	2.23954200
C	4.05894400	-0.88521200	0.17511800
H	4.88393400	-0.73718200	-1.91847500
H	4.94396800	-0.73012300	2.23899000
Be	1.32327300	-1.77020500	-1.15255000
Be	2.79718300	0.28640500	-0.62095300
Be	0.87179100	2.03096300	-1.15260800
Be	-0.47383100	-1.08196200	-1.92408800
Be	-1.64563600	2.27906500	-0.62038100
Be	-1.15109200	-2.56437500	-0.61985800
Be	-2.19456400	-0.26044500	-1.15292400
Be	1.17427200	0.13066400	-1.92427300
Be	-0.69994200	0.95169500	-1.92433600

10. Be$_{10}$@[6]CPP

C	2.82511400	-3.05290000	0.21551900
C	3.54805900	-2.74940700	-1.04583600
C	4.25698800	-1.53383600	-1.06105900
C	4.41239700	-0.74996300	0.11120400
C	4.26889400	-1.49430500	1.35871100
C	3.55335600	-2.64090600	1.41405300
H	3.58579500	-3.44082600	-1.87794100
H	4.62328200	-1.16695000	-2.01612200
H	4.73795400	-1.10892500	2.25656600
H	3.48078100	-3.20725500	2.33538200
C	1.47213800	-3.42167400	0.17519600
C	0.67477700	-3.52932800	1.37978700
C	0.76032000	-3.37978800	-1.12941300
C	-0.67541200	-3.52959400	1.37973400
H	1.19579800	-3.58051500	2.32871300
C	-0.76067700	-3.37958400	-1.12943500
H	1.18056900	-3.99279600	-1.92115800
C	-1.47268100	-3.42195600	0.17509400
H	-1.19651200	-3.58099800	2.32861100
H	-1.18103500	-3.99201000	-1.92157300
C	-2.82562600	-3.05267700	0.21529100
C	-3.54799700	-2.74866900	-1.04617300
C	-3.55419000	-2.64068800	1.41365000
C	-4.25692800	-1.53310100	-1.06142500
H	-3.58503300	-3.43957400	-1.87872500
C	-4.26974800	-1.49407400	1.35831300
H	-3.48183200	-3.20710000	2.33495600

C	-4.41302900	-0.74951300	0.11094800
H	-4.62283200	-1.16613900	-2.01660600
H	-4.73895600	-1.10885200	2.25616100
C	4.41235000	0.74941100	0.11117000
C	4.26917000	1.49392000	1.35859900
C	4.25729700	1.53333300	-1.06118800
C	3.55387600	2.64068100	1.41387500
H	4.73822000	1.10853600	2.25645900
C	3.54841800	2.74877400	-1.04593800
H	4.62393700	1.16663000	-2.01618300
C	2.82559100	3.05258200	0.21534100
H	3.48143700	3.20714500	2.33513900
H	3.58548200	3.43979300	-1.87840200
C	-1.47217000	3.42229600	0.17492700
C	-0.76017500	3.37959900	-1.12959900
C	-0.67485600	3.53027300	1.37949100
C	0.76077600	3.37947800	-1.12954100
H	-1.18048600	3.99184300	-1.92190700
C	0.67535200	3.52993200	1.37953100
H	-1.19591900	3.58213200	2.32836100
C	1.47266600	3.42173100	0.17498800
H	1.18124400	3.99189000	-1.92163700
H	1.19639000	3.58150400	2.32842700
C	-2.82512100	3.05289800	0.21529400
C	-3.55345600	2.64089900	1.41378300
C	-3.54776400	2.74899100	-1.04600200
C	-4.26902700	1.49430000	1.35848700
H	-3.48081000	3.20718700	2.33513800
C	-4.25720200	1.53382000	-1.06126200
H	-3.58442600	3.43982600	-1.87863200
C	-4.41274400	0.74995200	0.11102400
H	-4.73796400	1.10894800	2.25642200
H	-4.62376500	1.16723200	-2.01633100
Be	-1.88643900	-1.87797600	-0.92715800
Be	1.88697800	-1.87829800	-0.92903800
Be	-1.88584100	1.87805300	-0.92667300
Be	1.88677000	1.87753000	-0.92802600
Be	0.00007000	-1.71557100	-1.60777800
Be	-0.98708900	0.00002400	-1.09158200
Be	0.00034400	1.71542800	-1.60810200
Be	0.98755500	-0.00023800	-1.09464200
Be	-2.72767500	-0.00000400	-0.24577900
Be	2.72688700	-0.00049400	-0.24571500

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