

Electronic Supplementary Information (ESI)

Zigzag Double-Chain C-Be Nanoribbon Featuring Planar Pentacoordinate Carbon and Ribbon Aromaticity

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Contents

- SI1:** Fig. S1. The NBO results, including Wiberg bond indices of C–Be, Be–Be and Be–H bonds (WBI_{C-Be} , WBI_{Be-Be} , WBI_{Be-H} , in black font), total Wiberg bond indices of C, Be and H atoms (WBI_C , WBI_{Be} , WBI_H , in red font) and the natural charges (Q_C , Q_{Be} , Q_H , in blue font) of **3–5** at the B3LYP/cc-pVTZ level.
- SI2:** Fig. S2–S5. Full set of AdNDP orbitals of **1** and **3–5**.
- SI3:** Fig. S6. The comparison of the optimized geometries of **1–3** at B3LYP/cc-pVTZ, M06-2X/cc-pVTZ and B2PLYP-D3/cc-pVTZ levels and that of **4** and **5** at B3LYP/cc-pVTZ and M06-2X/cc-pVTZ levels. The point groups and the lowest vibrational frequencies (in cm^{-1}) are given in parenthesis.
- SI4:** B3LYP/cc-pVTZ optimized geometries (in Cartesian coordinates) and the CCSD(T) single-point energies + $ZPE_{B3LYP/cc-pVTZ}$ (in Hartree) of lowest-lying isomers (**2** and **2a–2e**) on $C_2Be_8H_6^{2+}$ potential energy surface.
- SI5:** Optimized geometries (in Cartesian coordinates) of **1–3** at B3LYP/cc-pVTZ, M06-2X/cc-pVTZ and B2PLYP-D3/cc-pVTZ levels and those of **4** and **5** at B3LYP/cc-pVTZ and M06-2X/cc-pVTZ levels.
- SI6:** Full form of Reference 60 and 61.

S11:

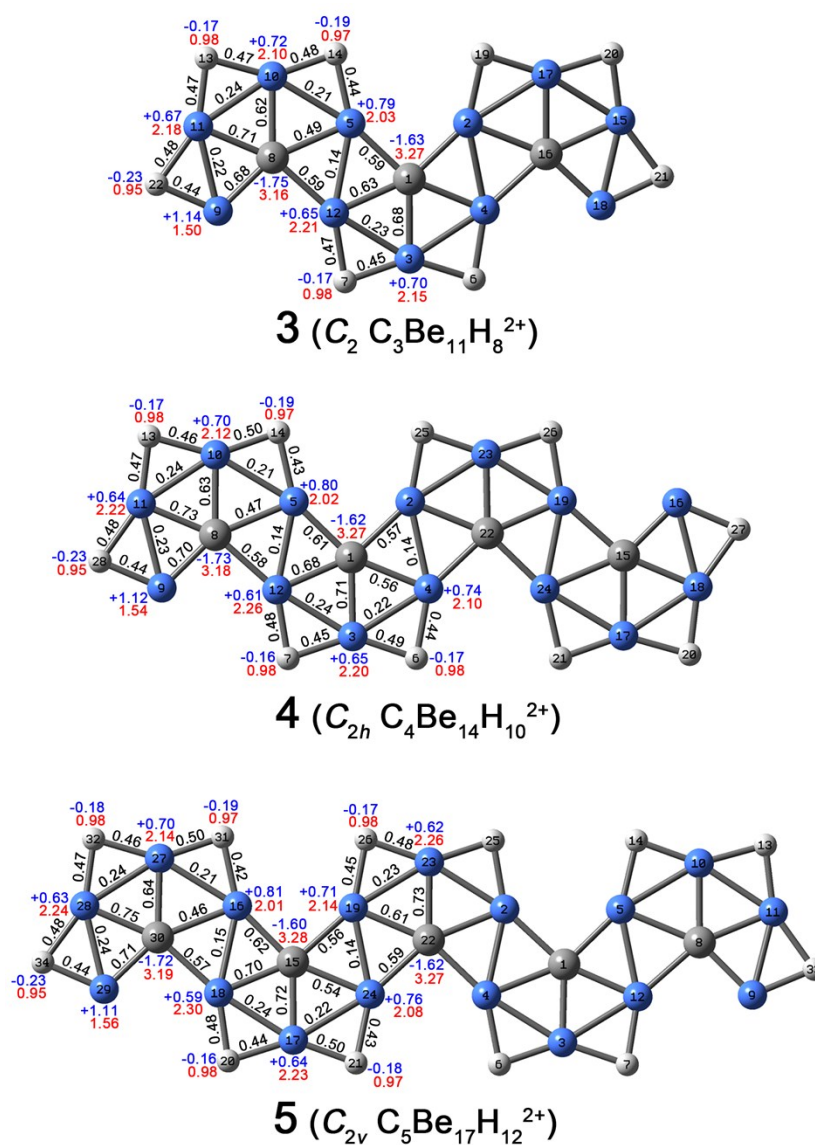


Figure S1. The NBO results, including Wiberg bond indices of C–Be, Be–Be and Be–H bonds (WBI_{C-Be} , WBI_{Be-Be} , WBI_{Be-H} , in black font), total Wiberg bond indices of C, Be and H atoms (WBI_C , WBI_{Be} , WBI_H , in red font) and the natural charges (Q_C , Q_{Be} , Q_H , in blue font) of **1–5** at the B3LYP/cc-pVTZ level.

S12: Figure S2-S5. Full set of AdNDP orbitals of **1** and **3–5**.

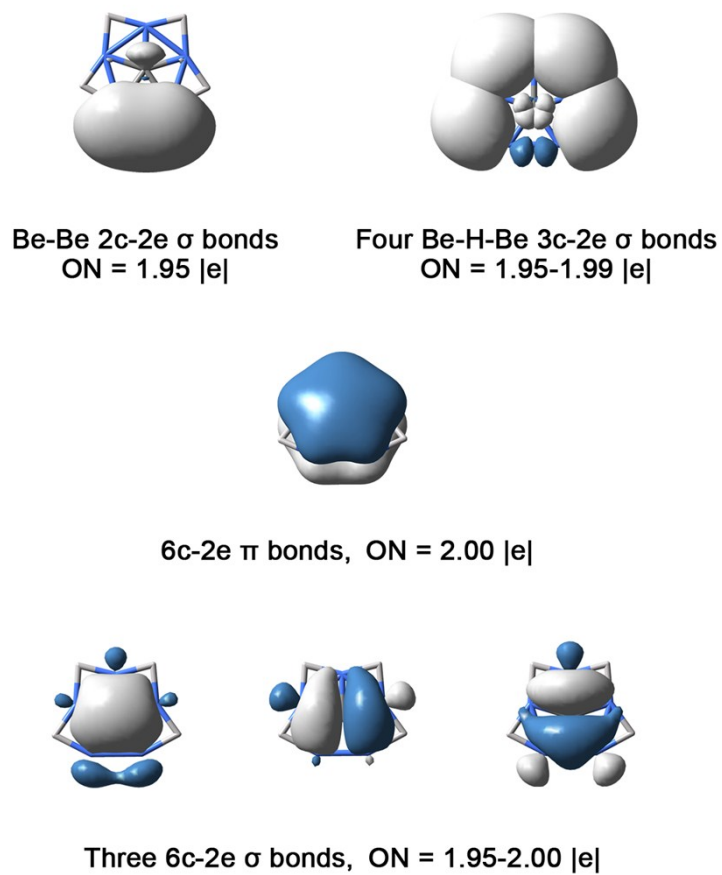
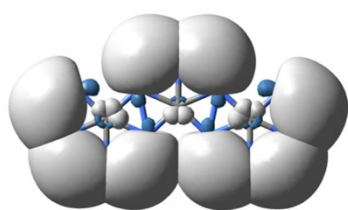
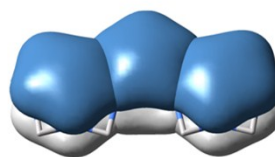


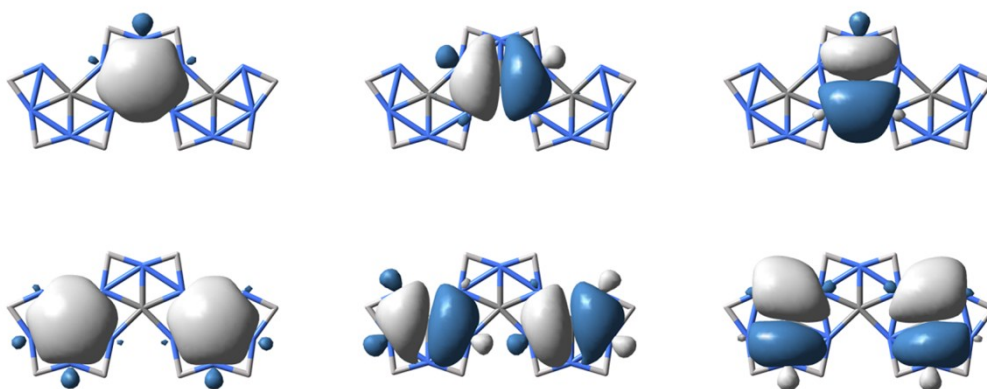
Figure S2. Full set of AdNDP orbitals of **1** (C_s CBe_5H_4).



Eight Be-H-Be 3c-2e σ bonds
ON = 1.97-1.99 |e|

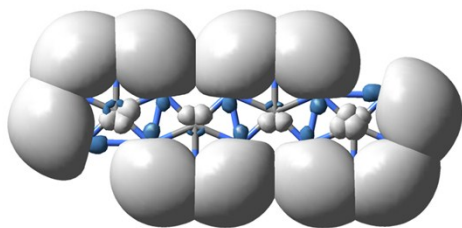


Three 6c-2e π bonds
ON = 1.97-1.99 |e|

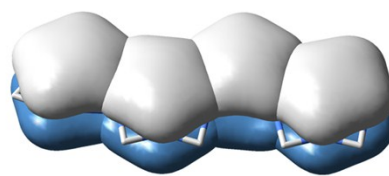


Nine 6c-2e σ bonds, ON = 1.94-1.99 |e|

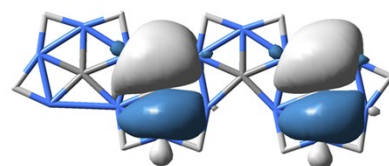
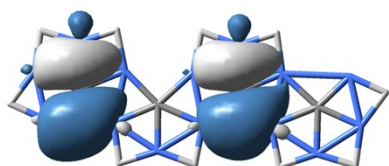
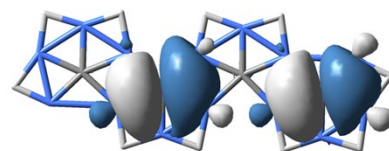
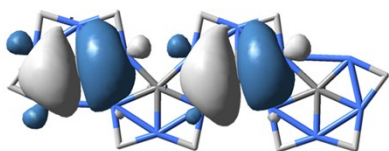
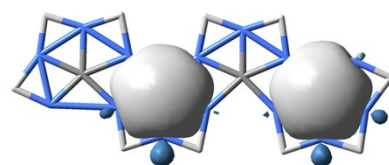
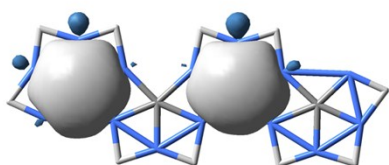
Figure S3. Full set of AdNDP orbitals of **3** (C_{2v} , $C_3Be_{11}H_8^{2+}$).



Ten Be-H-Be 3c-2e σ bonds
ON = 1.97-1.99 |e|

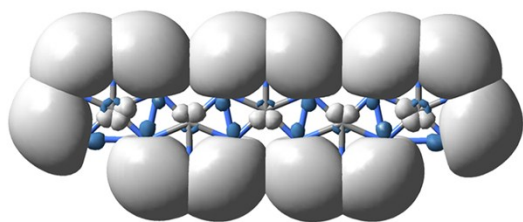


Four 6c-2e π bonds
ON = 1.97-2.00 |e|

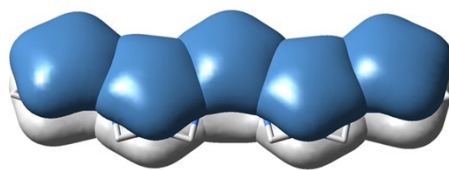


Twelve 6c-2e σ bonds, ON = 1.94-1.99 |e|

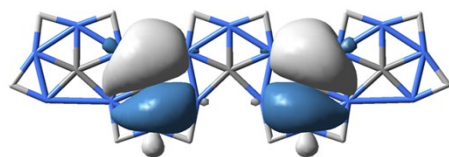
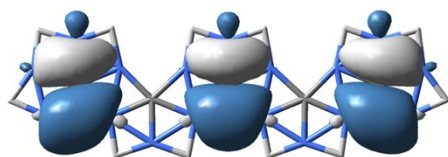
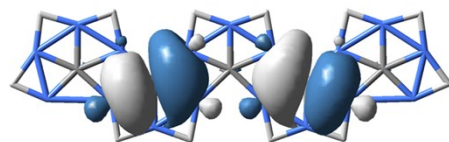
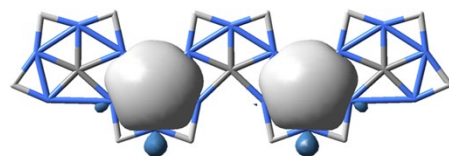
Figure S4. Full set of AdNDP orbitals of **4** (C_{2h} $C_4Be_{14}H_{10}^{2+}$).



Twelve Be-H-Be 3c-2e σ bonds
ON = 1.97-1.99 |e|



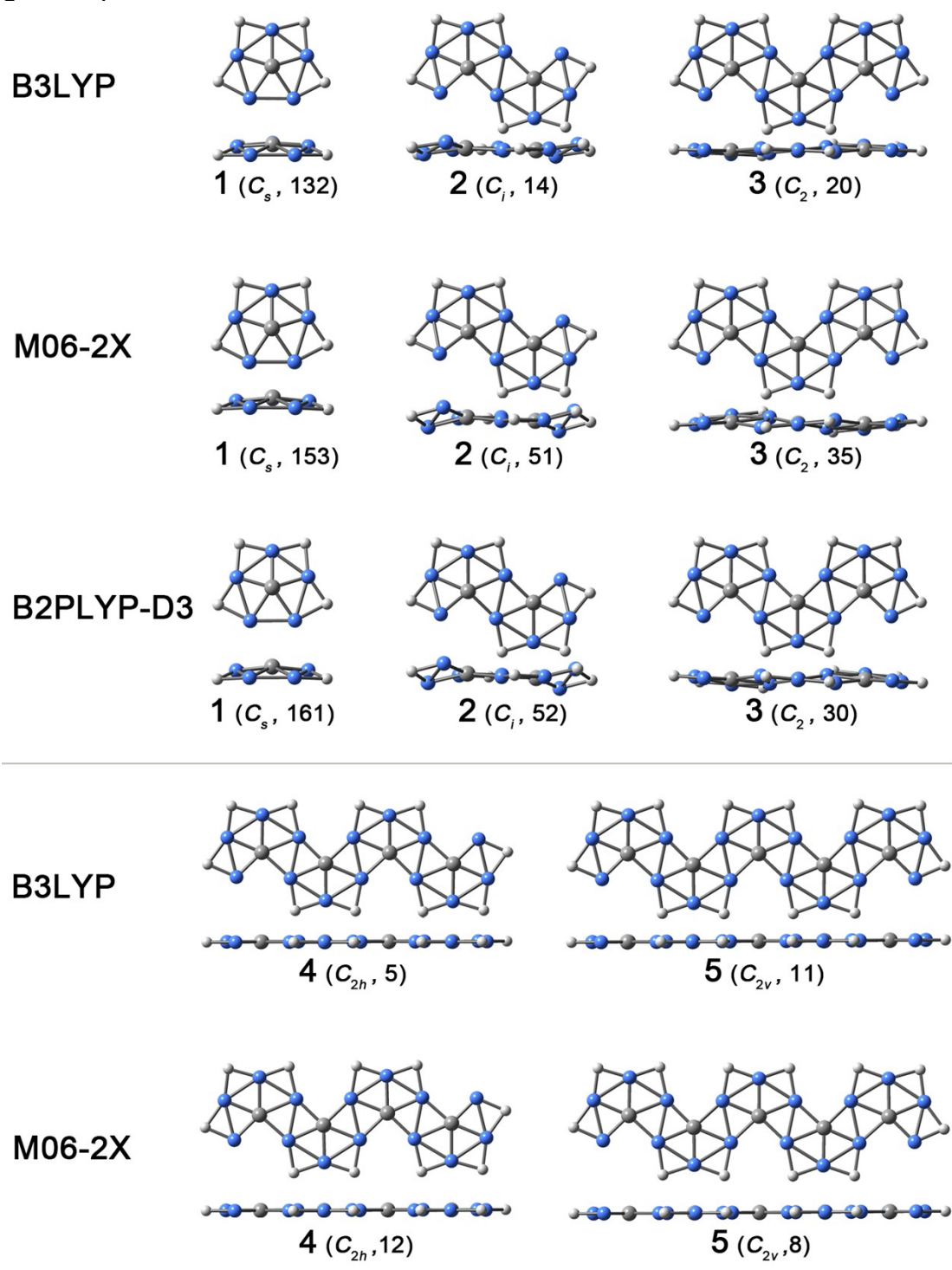
Five 6c-2e π bonds
ON = 1.97-2.00 |e|



Fifteen 6c-2e σ bonds, ON = 1.94-1.99 |e|

Figure S5. Full set of AdNDP orbitals of **5** (C_{2v} $C_5Be_{17}H_{12}^{2+}$).

SI3: Fig. S6. The comparison of the optimized geometries of **1–3** at B3LYP/cc-pVTZ, M06-2X/cc-pVTZ and B2PLYP-D3/cc-pVTZ levels and that of **4** and **5** at B3LYP/cc-pVTZ and M06-2X/cc-pVTZ levels. The point groups and the lowest vibrational frequencies (in cm^{-1}) are given in parenthesis.



S14: The B3LYP/cc-pVTZ optimized geometries (in Cartesian coordinates) and the CCSD(T) single-point energies + $\text{ZPE}_{\text{B3LYP/cc-pVTZ}}$ (in Hartree) of lowest-lying isomers (**2** and **2a–2e**) on $\text{C}_2\text{Be}_8\text{H}_6^{2+}$ potential energy surface.

2 ($E_{\text{CCSD(T)}} + \text{ZPE}_{\text{B3LYP}} = -196.6008367$ Hartree)

Coordinates:

C	1.445760	-0.233737	-0.026344
Be	2.632187	0.846190	-0.173250
Be	1.456812	-1.951051	-0.104932
Be	3.025398	-0.924485	0.193920
Be	0.182985	0.940306	0.108086
H	2.834012	-2.349256	0.093142
H	0.085116	-2.387957	-0.155492
C	-1.445760	0.233737	0.026344
Be	-2.632187	-0.846190	0.173250
Be	-1.456812	1.951051	0.104932
Be	-3.025398	0.924485	-0.193920
Be	-0.182985	-0.940306	-0.108086
H	-2.834012	2.349256	-0.093142
H	-0.085116	2.387957	0.155492
H	-3.913931	-0.257289	-0.024571
H	3.913931	0.257289	0.024571

2a ($E_{\text{CCSD(T)}} + \text{ZPE}_{\text{B3LYP}} = -196.5972208$ Hartree)

Coordinates:

H	-0.952179	0.417887	2.159774
H	-0.952179	0.417887	-2.159774
H	1.798518	4.466033	0.000000
H	-0.188954	-3.721225	0.000000
H	-0.580811	-2.150998	2.203983
H	-0.580811	-2.150998	-2.203983
Be	-0.020582	-2.639312	-0.957160
Be	1.137428	3.335527	0.000000
Be	-0.538697	-0.851200	-1.531838
Be	-0.538697	1.501237	1.330259
Be	0.797331	0.308236	0.000000
Be	-0.020582	-2.639312	0.957160
Be	-0.538697	-0.851200	1.531838
Be	-0.538697	1.501237	-1.330259
C	0.281241	1.889070	0.000000
C	0.135624	-1.212309	0.000000

2b ($E_{\text{CCSD(T)}} + \text{ZPE}_{\text{B3LYP}} = -196.5887762$ Hartree)

Coordinates:

C	0.000000	1.474466	0.252508
Be	0.918927	2.553808	1.015497

Be	-1.169288	1.616212	-1.008475
Be	-0.616360	3.081164	0.086132
Be	0.000000	0.000000	-0.976886
H	-1.534702	3.037350	-1.018509
H	-1.158331	0.465341	-1.813226
C	0.000000	-1.474466	0.252508
Be	-0.918927	-2.553808	1.015497
Be	1.169288	-1.616212	-1.008475
Be	0.616360	-3.081164	0.086132
Be	0.000000	0.000000	1.001457
H	1.534702	-3.037350	-1.018509
H	1.158331	-0.465341	-1.813226
H	-0.369012	-3.869725	0.894931
H	0.369012	3.869725	0.894931

2c ($E_{\text{CCSD(T)}} + \text{ZPE}_{\text{B3LYP}} = -196.5842923$ Hartree)

Coordinates:

C	-0.118108	1.944503	0.000000
C	0.055833	-1.371123	0.000000
Be	1.198866	-2.667563	0.000000
Be	-0.612352	3.173574	0.930067
Be	-0.612352	0.263082	0.000000
Be	1.650327	-0.848364	0.000000
Be	-1.657848	-1.360490	0.000000
Be	-0.659823	-2.954355	0.000000
Be	1.373174	1.372534	0.000000
H	2.382695	0.419260	0.000000
H	-2.102530	-0.031809	0.000000
H	-2.086091	-2.745693	0.000000
H	0.437320	-3.894384	0.000000
H	2.491170	-2.046545	0.000000
Be	-0.612352	3.173574	-0.930067
H	-1.019481	4.250919	0.000000

2d ($E_{\text{CCSD(T)}} + \text{ZPE}_{\text{B3LYP}} = -196.583805$ Hartree)

Coordinates:

H	4.210654	-0.738088	-0.405762
H	-3.315505	-1.763103	0.620959
H	0.468712	2.011690	0.706667
H	-1.672965	2.278201	-0.504754
H	2.972959	1.637548	0.594772
H	-3.664095	0.446179	-1.011364
Be	0.172959	-0.643118	-0.126184
Be	-0.727225	1.418514	0.258661
Be	2.938898	-1.360004	-0.627489
Be	-2.029324	-1.324247	1.067720
Be	1.590196	1.141983	0.442741
Be	-2.377967	1.065648	-0.713593

Be	3.270734	0.309515	0.126833
Be	-3.043017	-0.700521	-0.396221
C	1.756175	-0.420022	-0.118126
C	-1.452971	-0.163896	0.096394

2e ($E_{\text{CCSD(T)}} + \text{ZPE}_{\text{B3LYP}} = -196.5798689$ Hartree)

Coordinates:

C	-1.311632	0.176412	0.134296
C	1.648237	-0.184327	0.060705
Be	-2.940306	0.228322	-0.448090
Be	3.089535	-0.083447	-0.649927
Be	2.084579	1.449188	-0.246682
Be	-1.685762	-1.117248	-0.941642
Be	1.608443	-1.336792	1.185853
Be	-0.033320	-1.120747	0.117115
Be	0.231573	0.902754	0.058379
H	0.895709	2.223400	-0.227814
H	3.446423	1.287516	-0.858472
H	0.443325	-2.047949	1.349402
H	-0.606991	-2.019964	-0.950718
H	-3.092099	-0.925767	-1.293431
Be	-2.238150	1.159112	1.004469
H	-3.572366	1.205681	0.493128

SI5: Optimized geometries (in Cartesian coordinates) of **1–3** at B3LYP/cc-pVTZ, M06-2X/cc-pVTZ and B2PLYP-D3/cc-pVTZ levels and those of **4** and **5** at B3LYP/cc-pVTZ and M06-2X/cc-pVTZ levels.

1 (C_s CBe₅H₄)

Coordinates at B3LYP/cc-pVTZ level:

Be	0.00707700	-1.46997900	0.96693600
Be	0.00707700	0.43218800	1.54925500
Be	0.06755000	1.56560600	0.00000000
Be	0.00707700	0.43218800	-1.54925500
Be	0.00707700	-1.46997900	-0.96693600
H	0.22301900	1.92470500	1.42828100
H	0.22301900	1.92470500	-1.42828100
H	0.15240800	-0.74116500	2.36089000
H	0.15240800	-0.74116500	-2.36089000
C	-0.18904800	-0.05452900	0.00000000

Coordinates at M06-2X/cc-pVTZ level:

Be	0.01171000	-1.46753600	0.96123300
Be	0.01171000	0.43071900	1.54728300
Be	0.06784000	1.56482200	0.00000000
Be	0.01171000	0.43071900	-1.54728300
Be	0.01171000	-1.46753600	-0.96123300
H	0.25086100	1.91506700	1.42387700
H	0.25086100	1.91506700	-1.42387700
H	0.18264100	-0.74338300	2.34857600
H	0.18264100	-0.74338300	-2.34857600
C	-0.22095500	-0.05135400	0.00000000

Coordinates at B2PLYP-D3/cc-pVTZ level:

Be	0.01184200	-1.46901300	0.96727000
Be	0.01184200	0.43202600	1.54875400
Be	0.07321800	1.56597400	0.00000000
Be	0.01184200	0.43202600	-1.54875400
Be	0.01184200	-1.46901300	-0.96727000
H	0.27108300	1.91524100	1.42424000
H	0.27108300	1.91524100	-1.42424000
H	0.19535800	-0.74060400	2.35182500
H	0.19535800	-0.74060400	-2.35182500
C	-0.23587100	-0.05287900	0.00000000

2 (C_i C₂Be₈H₆²⁺)

Coordinates at B3LYP/cc-pVTZ level:

C	1.445760	-0.233737	-0.026344
Be	2.632187	0.846190	-0.173250
Be	1.456812	-1.951051	-0.104932
Be	3.025398	-0.924485	0.193920

Be	0.182985	0.940306	0.108086
H	2.834012	-2.349256	0.093142
H	0.085116	-2.387957	-0.155492
C	-1.445760	0.233737	0.026344
Be	-2.632187	-0.846190	0.173250
Be	-1.456812	1.951051	0.104932
Be	-3.025398	0.924485	-0.193920
Be	-0.182985	-0.940306	-0.108086
H	-2.834012	2.349256	-0.093142
H	-0.085116	2.387957	0.155492
H	-3.913931	-0.257289	-0.024571
H	3.913931	0.257289	0.024571

Coordinates at M06-2X/cc-pVTZ level:

C	1.44135000	-0.21646800	-0.05624600
Be	2.65996700	0.79855700	-0.34777600
Be	1.47949400	-1.92512000	-0.19392800
Be	2.98437200	-0.89743500	0.34220800
Be	0.17560000	0.93656100	0.16943300
H	2.82554700	-2.31844700	0.16739000
H	0.11903000	-2.37883700	-0.26014300
C	-1.44135000	0.21646800	0.05624600
Be	-2.65996700	-0.79855700	0.34777600
Be	-1.47949400	1.92512000	0.19392800
Be	-2.98437200	0.89743500	-0.34220800
Be	-0.17560000	-0.93656100	-0.16943300
H	-2.82554700	2.31844700	-0.16739000
H	-0.11903000	2.37883700	0.26014300
H	-3.91216100	-0.21842100	-0.00729900
H	3.91216100	0.21842100	0.00729900

Coordinates at B2PLYP-D3/cc-pVTZ level:

C	1.44303400	-0.21868900	-0.05635400
Be	2.65891600	0.81046300	-0.32290200
Be	1.47724900	-1.93458000	-0.19000400
Be	2.99909400	-0.90407300	0.32433900
Be	0.17845900	0.94049800	0.15368500
H	2.82981600	-2.32694400	0.15397900
H	0.11161000	-2.38439200	-0.23946400
C	-1.44303400	0.21868900	0.05635400
Be	-2.65891600	-0.81046300	0.32290200
Be	-1.47724900	1.93458000	0.19000400
Be	-2.99909400	0.90407300	-0.32433900
Be	-0.17845900	-0.94049800	-0.15368500
H	-2.82981600	2.32694400	-0.15397900
H	-0.11161000	2.38439200	0.23946400
H	-3.91799300	-0.22723200	-0.01399500
H	3.91799300	0.22723200	0.01399500

3 ($C_2 C_3 Be_{11} H_4^{2+}$)

Coordinates at B3LYP/cc-pVTZ level:

C	0.00000000	0.00000000	0.44538600
Be	0.11210000	-1.22441300	-0.73221200
Be	0.00000000	0.00000000	2.13023200
Be	-0.09197800	-1.60212700	1.12698000
Be	-0.11210000	1.22441300	-0.73221200
H	-0.06730400	-1.36821600	2.58164800
H	0.06730400	1.36821600	2.58164800
C	0.00000000	2.88738200	-0.04251600
Be	0.04085900	4.04434700	1.06146700
Be	-0.15357700	2.87386600	-1.74218500
Be	0.04359000	4.45962800	-0.72907700
Be	0.09197800	1.60212700	1.12698000
H	-0.09699000	4.26772400	-2.14955000
H	-0.23722000	1.52433700	-2.18890000
Be	-0.04359000	-4.45962800	-0.72907700
C	0.00000000	-2.88738200	-0.04251600
Be	0.15357700	-2.87386600	-1.74218500
Be	-0.04085900	-4.04434700	1.06146700
H	0.23722000	-1.52433700	-2.18890000
H	0.09699000	-4.26772400	-2.14955000
H	-0.08426100	-5.34298700	0.47538100
H	0.08426100	5.34298700	0.47538100

Coordinates at M06-2X/cc-pVTZ level:

C	0.00000000	0.00000000	0.45136200
Be	-0.21275800	-1.22042100	-0.71236300
Be	0.00000000	0.00000000	2.13395800
Be	0.17739700	-1.59218700	1.12182900
Be	0.21275800	1.22042100	-0.71236300
H	0.12962000	-1.36567500	2.57798100
H	-0.12962000	1.36567500	2.57798100
C	0.00000000	2.87668600	-0.04179000
Be	-0.02213900	4.05065300	1.04805200
Be	0.25415100	2.86322500	-1.72684100
Be	-0.13853900	4.43006300	-0.74914800
Be	-0.17739700	1.59218700	1.12182900
H	0.10609500	4.24307600	-2.15382700
H	0.41349700	1.51688600	-2.15957800
Be	0.13853900	-4.43006300	-0.74914800
C	0.00000000	-2.87668600	-0.04179000
Be	-0.25415100	-2.86322500	-1.72684100
Be	0.02213900	-4.05065300	1.04805200
H	-0.41349700	-1.51688600	-2.15957800
H	-0.10609500	-4.24307600	-2.15382700
H	0.15213000	-5.33239000	0.43804700
H	-0.15213000	5.33239000	0.43804700

Coordinates at B2PLYP-D3/cc-pVTZ level:

C	0.00000000	0.00000000	0.44926400
Be	0.18431400	-1.22008600	-0.72143400
Be	0.00000000	0.00000000	2.13830000
Be	-0.15369200	-1.59871900	1.12684900
Be	-0.18431400	1.22008600	-0.72143400
H	-0.11092000	-1.36862300	2.58303300
H	0.11092000	1.36862300	2.58303300
C	0.00000000	2.88155900	-0.04176800
Be	0.03975100	4.05256400	1.05540500
Be	-0.22634000	2.86643400	-1.73621500
Be	0.09767700	4.44994100	-0.74471300
Be	0.15369200	1.59871900	1.12684900
H	-0.11831200	4.25405300	-2.15583000
H	-0.36333100	1.51617400	-2.17164700
Be	-0.09767700	-4.44994100	-0.74471300
C	0.00000000	-2.88155900	-0.04176800
Be	0.22634000	-2.86643400	-1.73621500
Be	-0.03975100	-4.05256400	1.05540500
H	0.36333100	-1.51617400	-2.17164700
H	0.11831200	-4.25405300	-2.15583000
H	-0.13222900	-5.34305300	0.45109400
H	0.13222900	5.34305300	0.45109400

4 (C_{2h} $C_4Be_{14}H_{10}^{2+}$)

Coordinates at B3LYP/cc-pVTZ level:

C	-0.27897600	1.43894300	0.00000000
Be	0.92030600	0.21037500	0.00000000
Be	-1.95648800	1.38384900	0.00000000
Be	-0.92030600	-0.21037500	0.00000000
Be	0.87720400	2.67049000	0.00000000
H	-2.39266800	0.02822800	0.00000000
H	-2.44498100	2.74893700	0.00000000
C	0.14293000	4.33078600	0.00000000
Be	-0.99701800	5.44492000	0.00000000
Be	1.84155100	4.35203300	0.00000000
Be	0.77640600	5.91364400	0.00000000
Be	-0.99701800	3.00551500	0.00000000
H	2.20926300	5.76235000	0.00000000
H	2.33889000	3.02268000	0.00000000
C	-0.14293000	-4.33078600	0.00000000
Be	0.99701800	-5.44492000	0.00000000
Be	-1.84155100	-4.35203300	0.00000000
Be	-0.77640600	-5.91364400	0.00000000
Be	0.99701800	-3.00551500	0.00000000
H	-2.20926300	-5.76235000	0.00000000
H	-2.33889000	-3.02268000	0.00000000
C	0.27897600	-1.43894300	0.00000000
Be	1.95648800	-1.38384900	0.00000000

Be	-0.87720400	-2.67049000	0.00000000
H	2.39266800	-0.02822800	0.00000000
H	2.44498100	-2.74893700	0.00000000
H	0.45717000	-6.76504100	0.00000000
H	-0.45717000	6.76504100	0.00000000

Coordinates at M06-2X/cc-pVTZ level:

C	-0.28713700	1.43380800	0.00000000
Be	0.91938900	0.21260100	0.00000000
Be	-1.96329500	1.37387700	0.00000000
Be	-0.91938900	-0.21260100	0.00000000
Be	0.86804300	2.66470800	0.00000000
H	-2.39069400	0.01510300	0.00000000
H	-2.45046600	2.73961500	0.00000000
C	0.13543600	4.32089000	0.00000000
Be	-1.00552900	5.43674300	0.00000000
Be	1.83287000	4.34224600	0.00000000
Be	0.76958800	5.90005600	0.00000000
Be	-1.00552900	2.99475500	0.00000000
H	2.19991100	5.75056100	0.00000000
H	2.32785700	3.01315700	0.00000000
C	-0.13543600	-4.32089000	0.00000000
Be	1.00552900	-5.43674300	0.00000000
Be	-1.83287000	-4.34224600	0.00000000
Be	-0.76958800	-5.90005600	0.00000000
Be	1.00552900	-2.99475500	0.00000000
H	-2.19991100	-5.75056100	0.00000000
H	-2.32785700	-3.01315700	0.00000000
C	0.28713700	-1.43380800	0.00000000
Be	1.96329500	-1.37387700	0.00000000
Be	-0.86804300	-2.66470800	0.00000000
H	2.39069400	-0.01510300	0.00000000
H	2.45046600	-2.73961500	0.00000000
H	0.45754700	-6.75336700	0.00000000
H	-0.45754700	6.75336700	0.00000000

5 (C_{2v} $C_5Be_{17}H_{12}^{2+}$)

Coordinates at B3LYP/cc-pVTZ level:

C	0.00000000	2.88432900	-0.37472700
Be	0.00000000	1.61058500	0.79558200
Be	0.00000000	2.86142200	-2.04895700
Be	0.00000000	1.23481400	-1.05219800
Be	0.00000000	4.07355700	0.81295100
H	0.00000000	1.52395300	-2.52572500
H	0.00000000	4.24351200	-2.50582700
C	0.00000000	5.75981900	0.12247400
Be	0.00000000	6.89210100	-0.99459300
Be	0.00000000	5.73624500	1.81757000

Be	0.00000000	7.32281700	0.78754400
Be	0.00000000	4.45802500	-1.05193300
H	0.00000000	7.14136300	2.21800700
H	0.00000000	4.39999000	2.28859100
C	0.00000000	-2.88432900	-0.37472700
Be	0.00000000	-4.07355700	0.81295100
Be	0.00000000	-2.86142200	-2.04895700
Be	0.00000000	-4.45802500	-1.05193300
Be	0.00000000	-1.61058500	0.79558200
H	0.00000000	-4.24351200	-2.50582700
H	0.00000000	-1.52395300	-2.52572500
C	0.00000000	0.00000000	0.11960800
Be	0.00000000	0.00000000	1.79291000
Be	0.00000000	-1.23481400	-1.05219800
H	0.00000000	1.35294100	2.26086300
H	0.00000000	-1.35294100	2.26086300
Be	0.00000000	-5.73624500	1.81757000
Be	0.00000000	-7.32281700	0.78754400
Be	0.00000000	-6.89210100	-0.99459300
C	0.00000000	-5.75981900	0.12247400
H	0.00000000	-4.39999000	2.28859100
H	0.00000000	-7.14136300	2.21800700
H	0.00000000	8.20331200	-0.43089900
H	0.00000000	-8.20331200	-0.43089900

Coordinates at M06-2X/cc-pVTZ level:

C	0.00000000	2.87642700	-0.37978100
Be	0.00000000	1.60602800	0.79338600
Be	0.00000000	2.85363900	-2.05241400
Be	0.00000000	1.23196300	-1.05317900
Be	0.00000000	4.06249300	0.81006900
H	0.00000000	1.51520300	-2.52519400
H	0.00000000	4.23705700	-2.50456500
C	0.00000000	5.74608100	0.12445600
Be	0.00000000	6.88263900	-0.99036000
Be	0.00000000	5.71905500	1.81796900
Be	0.00000000	7.30375500	0.79377800
Be	0.00000000	4.44602200	-1.05313700
H	0.00000000	7.12088900	2.22055800
H	0.00000000	4.38287500	2.28416800
C	0.00000000	-2.87642700	-0.37978100
Be	0.00000000	-4.06249300	0.81006900
Be	0.00000000	-2.85363900	-2.05241400
Be	0.00000000	-4.44602200	-1.05313700
Be	0.00000000	-1.60602800	0.79338600
H	0.00000000	-4.23705700	-2.50456500
H	0.00000000	-1.51520300	-2.52519400
C	0.00000000	0.00000000	0.12155400
Be	0.00000000	0.00000000	1.79298900
Be	0.00000000	-1.23196300	-1.05317900

H	0.00000000	1.35453800	2.25702100
H	0.00000000	-1.35453800	2.25702100
Be	0.00000000	-5.71905500	1.81796900
Be	0.00000000	-7.30375500	0.79377800
Be	0.00000000	-6.88263900	-0.99036000
C	0.00000000	-5.74608100	0.12445600
H	0.00000000	-4.38287500	2.28416800
H	0.00000000	-7.12088900	2.22055800
H	0.00000000	8.18843200	-0.41513000
H	0.00000000	-8.18843200	-0.41513000

SI6: Full form of reference 60 and 61.

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