Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Viable aromatic Be_nH_n stars enclosing a planar hypercoordinate boron or late transition metal

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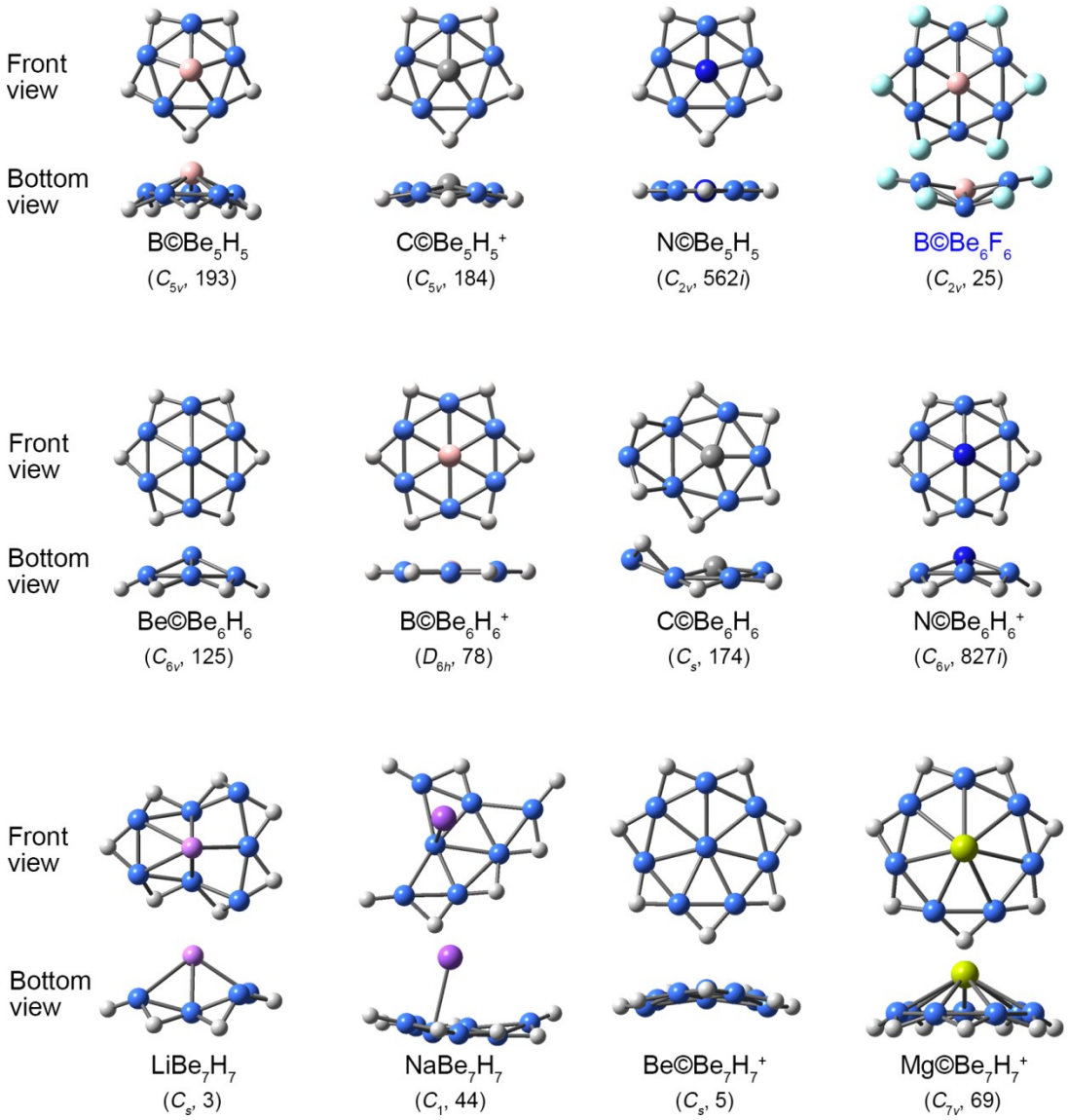

Fig. S1. Optimized structures, point groups, and the lowest vibrational frequencies (in cm^{-1}) of species with a Be_nH_n (n = 5, 6, 7) ring and center main group element, as well as those of $BBe_6F_6^+$.

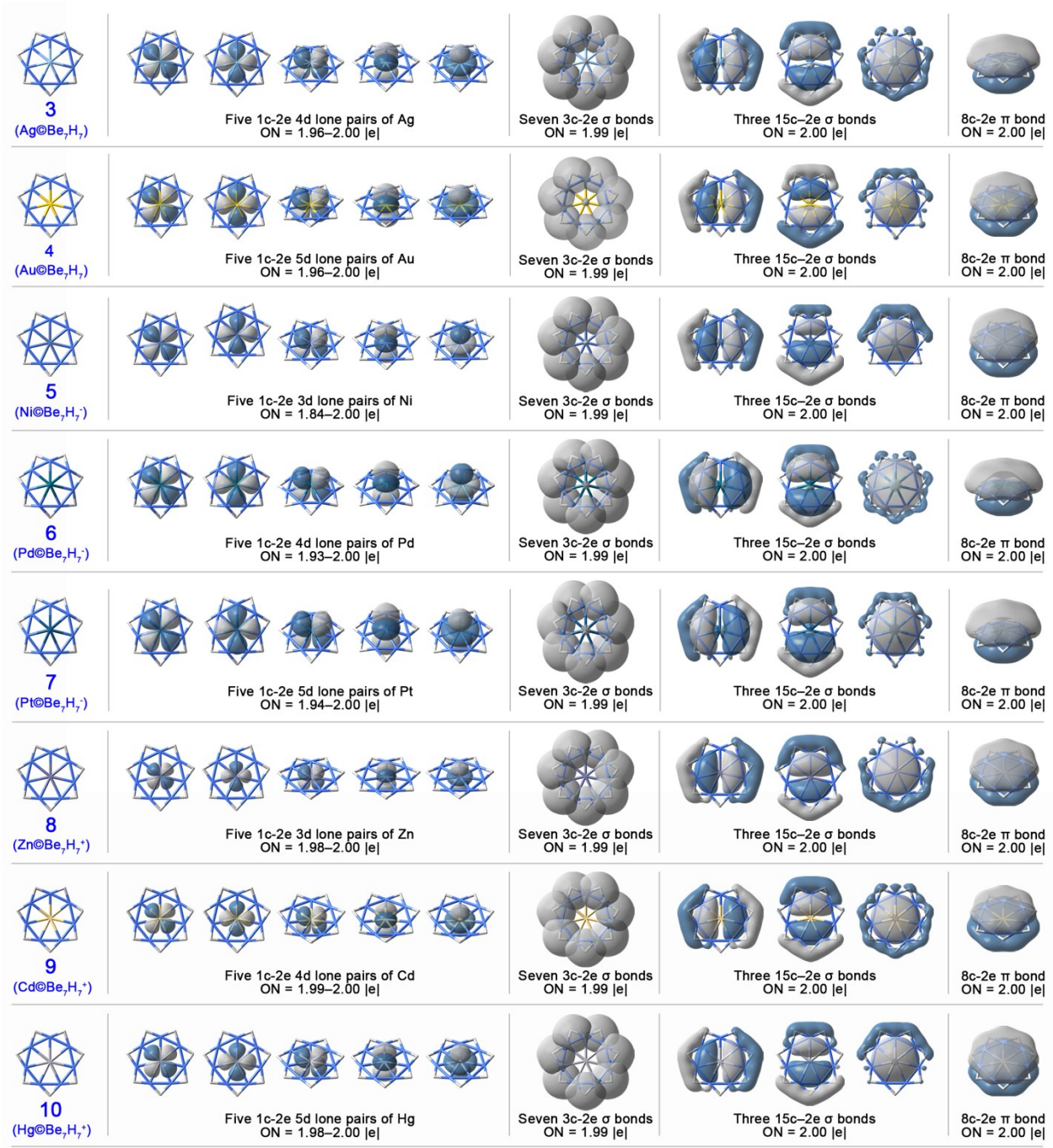

Fig. S2. The AdNDP results of **3~10** at the B3LYP level with 6-31G for Be and H and LANL2DZ for transition metals.

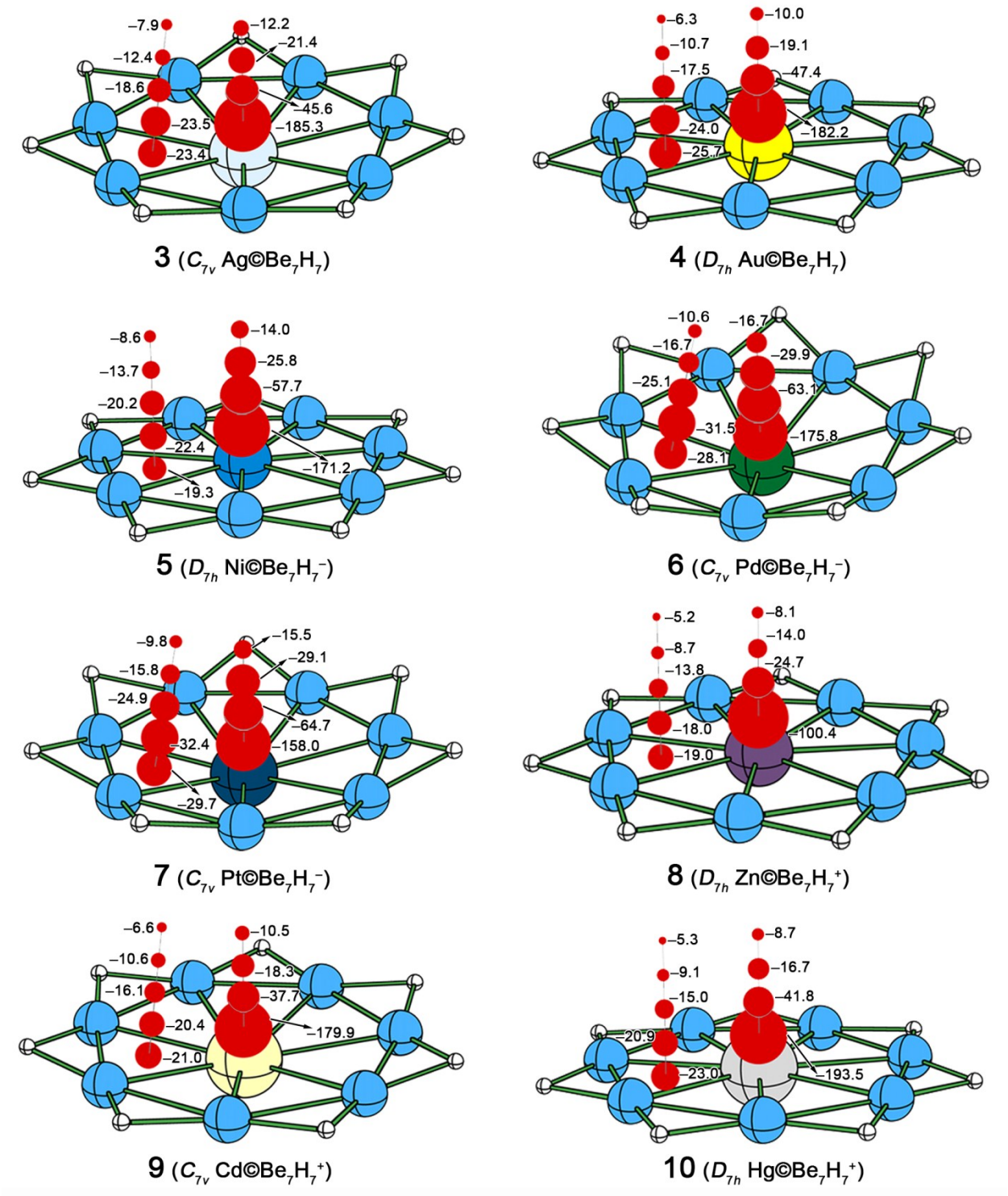

Fig. S3. The NICS calculation results of **3~10** at the B3LYP/BSI level.

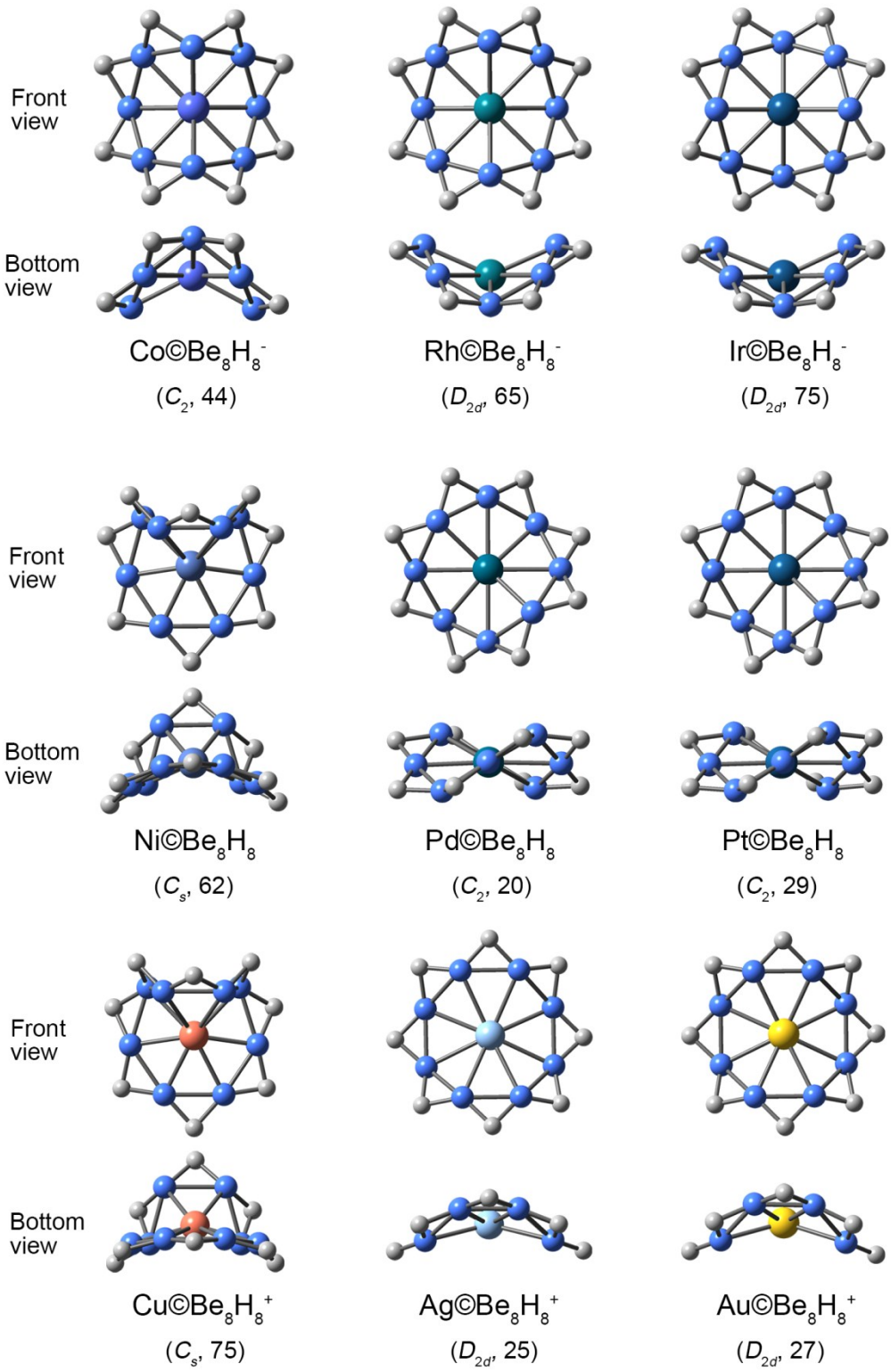

Fig. S4. Optimized structures, point groups, and the lowest vibrational frequencies (in cm^{-1}) of species with a Be_8H_8 star.

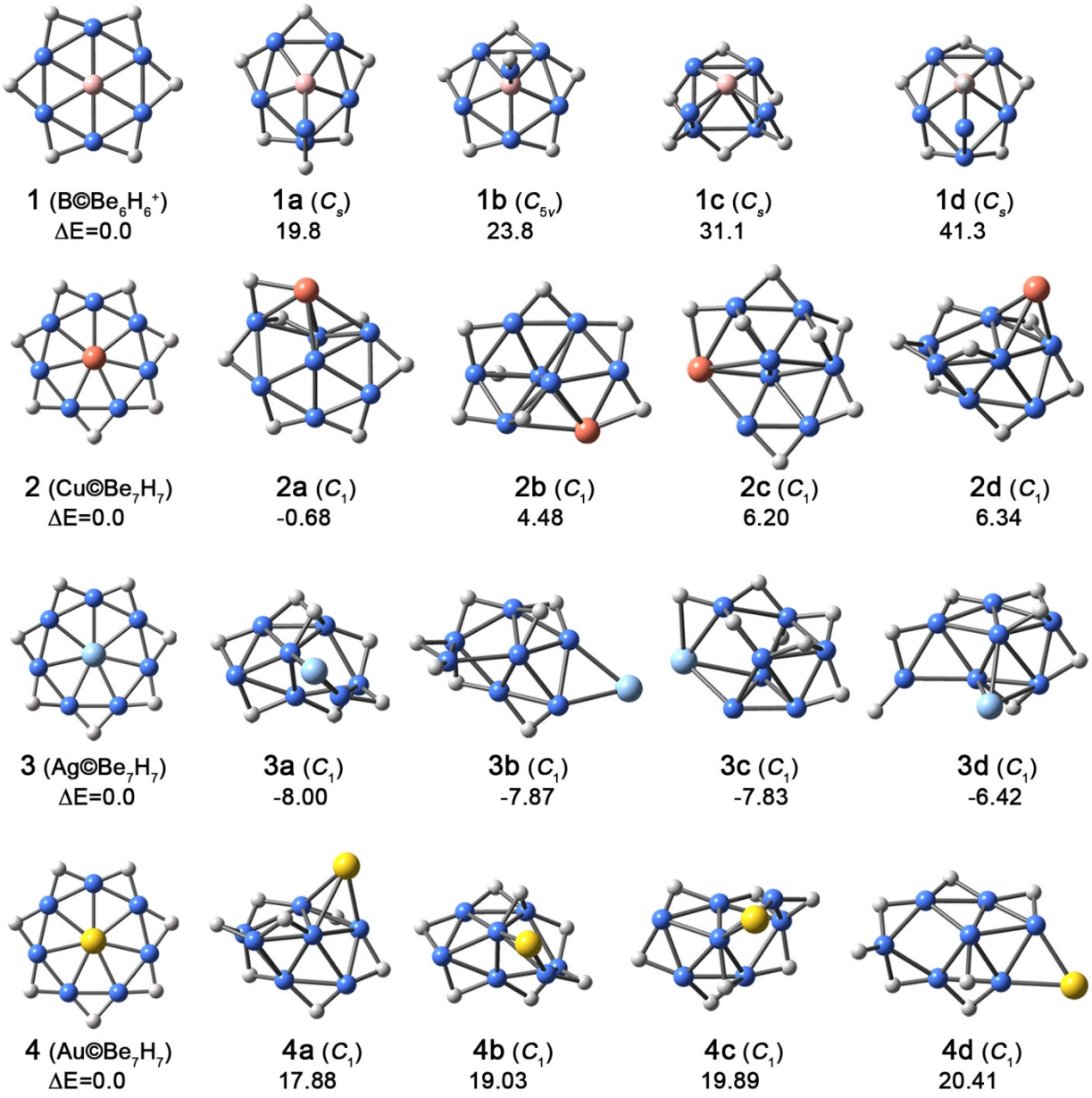

Fig. S5. B3LYP-optimized structures and CCSD(T) relative energies of five lowest isomers of $Be_6H_6B^+$, Be_7H_7Cu, Be_7H_7Ag, and Be_7H_7Au components.

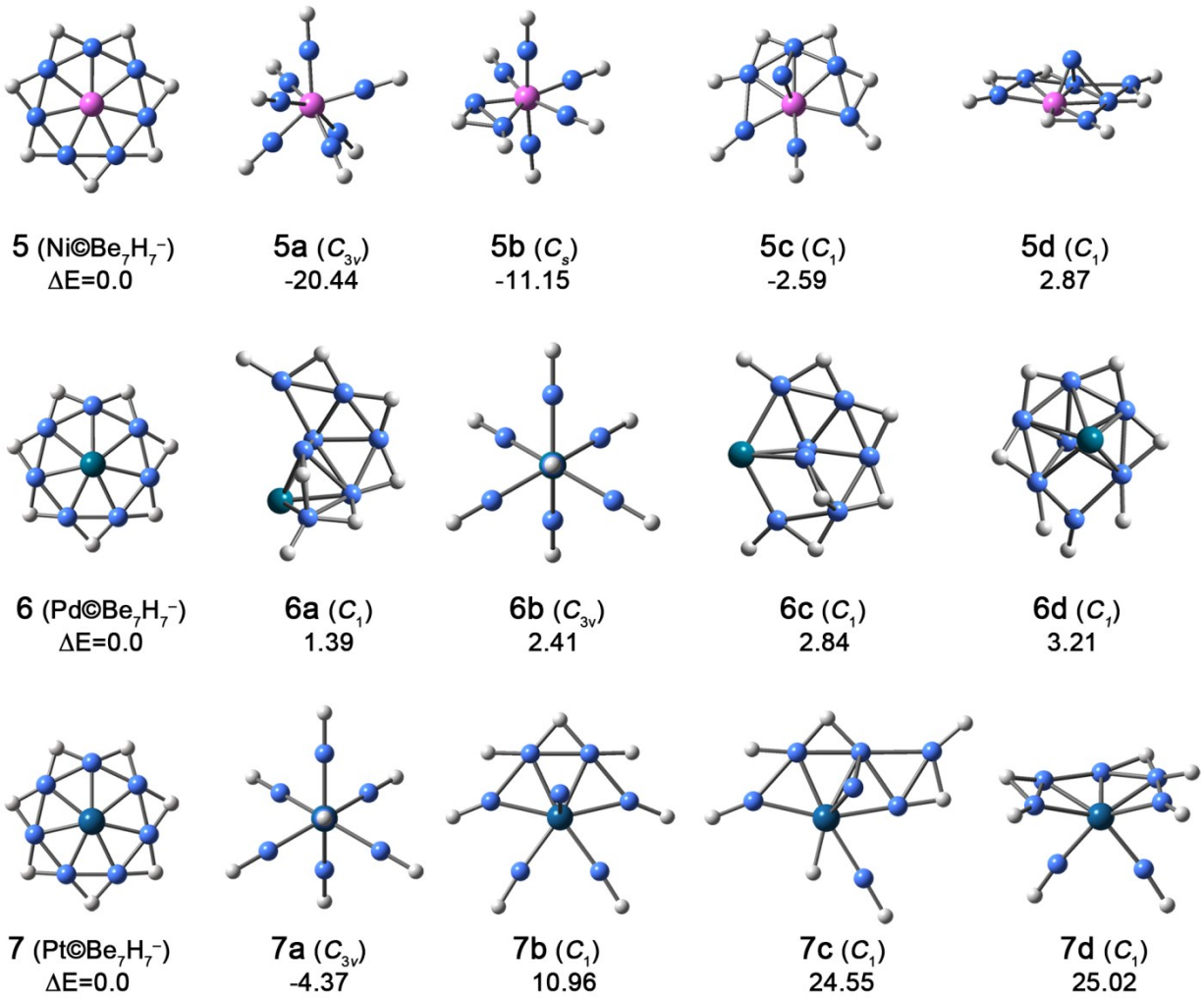

Fig. S6. B3LYP-optimized structures and CCSD(T) relative energies of five lowest isomers of $Be_7H_7Ni^-$, $Be_7H_7Pd^-$, and $Be_7H_7Pt^-$ components.

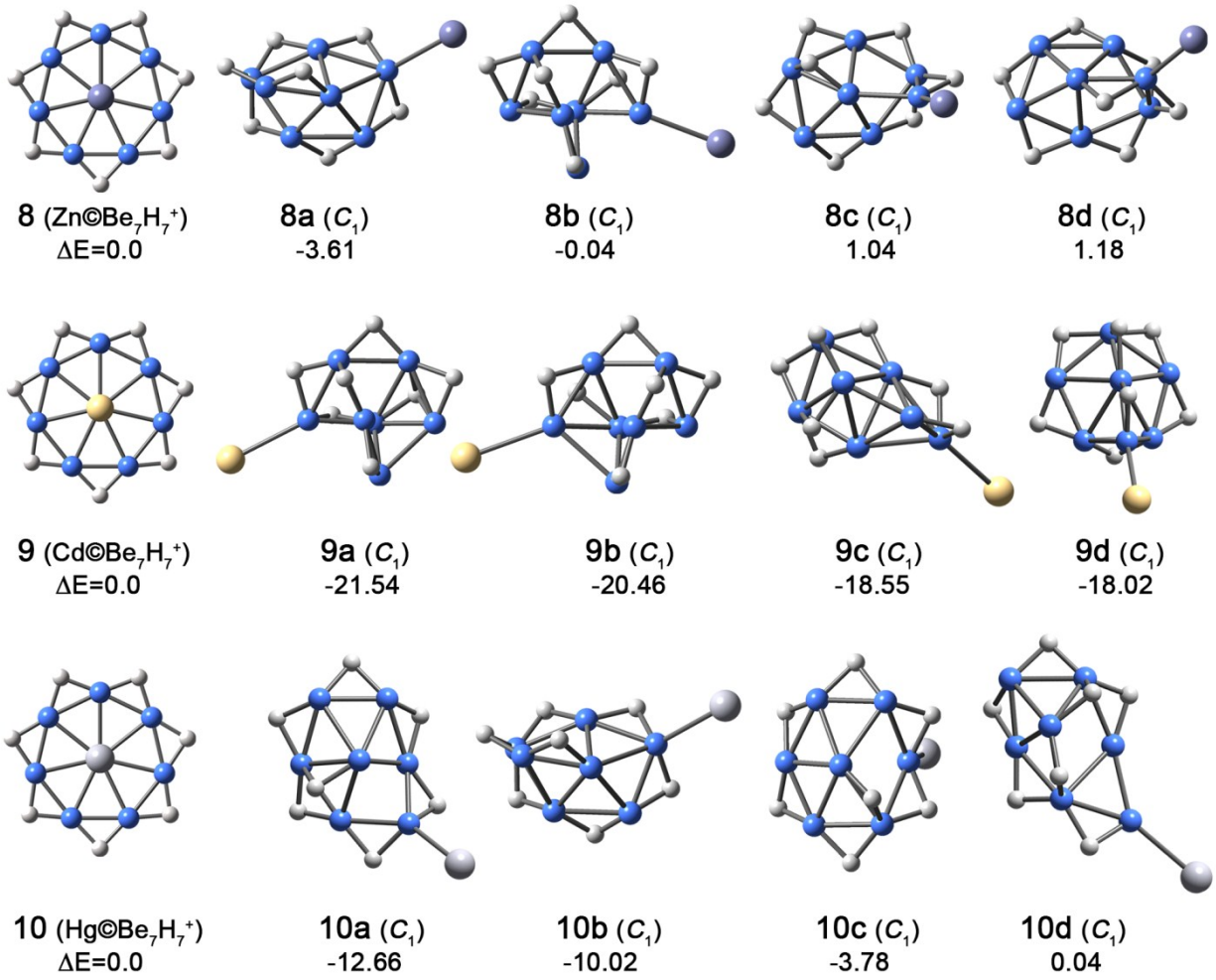

Fig. S7. B3LYP-optimized structures and CCSD(T) relative energies of five lowest isomers of $Be_7H_7Zn^+$, $Be_7H_7Cd^+$, and $Be_7H_7Hg^+$ components.

The Cartesian coordinates of B3LYP/BSI- and B2PLYP-D/BSI-optimized structures shown in Fig. 1 as well as those of B3LYP/BSI-optimized structure shown in Fig. S1, and Fig. S4~S7.

a. B2PLYP-D/BSI-optimized structures of molecules shown in Fig. 1.

$B©Be_6H_6^+$ (**1**)

H	2.730872	0.000000	0.000000
H	1.365436	2.365005	0.000000
H	-1.365436	2.365005	0.000000
H	-2.730872	0.000000	0.000000
H	-1.365436	-2.365005	0.000000
H	1.365436	-2.365005	0.000000
Be	0.000000	1.887101	0.000000
Be	1.634278	0.943551	0.000000
Be	-1.634278	0.943551	0.000000
Be	-1.634278	-0.943551	0.000000
Be	0.000000	-1.887101	0.000000
Be	1.634278	-0.943551	0.000000
B	0.000000	0.000000	0.000000

$Cu©Be_7H_7$ (**2**)

Be	0.000000	2.181853	0.000000
Be	-1.705841	1.360363	0.000000
Be	-2.127149	-0.485508	0.000000
Be	-0.946670	-1.965781	0.000000
Be	0.946670	-1.965781	0.000000
Be	1.705841	1.360363	0.000000
Be	2.127149	-0.485508	0.000000
H	1.335687	2.773582	0.000000
H	-1.335687	2.773582	0.000000
H	-3.001261	0.685018	0.000000
H	-2.406825	-1.919379	0.000000
H	0.000000	-3.078444	0.000000
H	3.001261	0.685018	0.000000
H	2.406825	-1.919379	0.000000
Cu	0.000000	0.000000	0.000000

Ag©Be_7H_7 (**3**)

Be	0.000000	2.249320	-0.152097
Be	1.758589	1.402428	-0.152097
Be	2.192925	-0.500521	-0.152097
Be	0.975943	-2.026567	-0.152097
Be	-0.975943	-2.026567	-0.152097
Be	-1.758589	1.402428	-0.152097
Be	-2.192925	-0.500521	-0.152097
H	-1.339834	2.782194	-0.435754
H	1.339834	2.782194	-0.435754
H	3.010580	0.687145	-0.435754
H	2.414298	-1.925338	-0.435754
H	0.000000	-3.088003	-0.435754
H	-3.010580	0.687145	-0.435754
H	-2.414298	-1.925338	-0.435754
Ag	0.000000	0.000000	0.155511

Au©Be_7H_7 (**4**)

Be	0.000000	2.248640	0.000000
Be	-1.758058	1.402004	0.000000
Be	-2.192262	-0.500370	0.000000
Be	-0.975648	-2.025955	0.000000
Be	0.975648	-2.025955	0.000000
Be	1.758058	1.402004	0.000000
Be	2.192262	-0.500370	0.000000
H	1.358430	2.820808	0.000000
H	-1.358430	2.820808	0.000000
H	-3.052364	0.696682	0.000000
H	-2.447806	-1.952060	0.000000
H	0.000000	-3.130861	0.000000
H	3.052364	0.696682	0.000000
H	2.447806	-1.952060	0.000000
Au	0.000000	0.000000	0.000000

Ni©$Be_7H_7^-$ (**5**)

Be	0.000000	2.178442	0.000000
Be	1.703175	1.358237	0.000000
Be	2.123824	-0.484749	0.000000
Be	0.945191	-1.962709	0.000000
Be	-0.945191	-1.962709	0.000000
Be	-1.703175	1.358237	0.000000

Be	-2.123824	-0.484749	0.000000
H	-1.345237	2.793413	0.000000
H	1.345237	2.793413	0.000000
H	3.022720	0.689916	0.000000
H	2.424033	-1.933102	0.000000
H	0.000000	-3.100455	0.000000
H	-3.022720	0.689916	0.000000
H	-2.424033	-1.933102	0.000000
Ni	0.000000	0.000000	0.000000

$Pd©Be_7H_7^-$ (**6**)

Be	0.000000	2.205087	-0.226947
Be	-1.724006	1.374849	-0.226947
Be	-2.149800	-0.490678	-0.226947
Be	-0.956751	-1.986714	-0.226947
Be	0.956751	-1.986714	-0.226947
Be	1.724006	1.374849	-0.226947
Be	2.149800	-0.490678	-0.226947
H	1.308776	2.717702	-0.692089
H	-1.308776	2.717702	-0.692089
H	-2.940794	0.671217	-0.692089
H	-2.358333	-1.880708	-0.692089
H	0.000000	-3.016422	-0.692089
H	2.940794	0.671217	-0.692089
H	2.358333	-1.880708	-0.692089
Pd	0.000000	0.000000	0.243460

$Pt©Be_7H_7^-$ (**7**)

Be	0.000000	2.205274	-0.242366
Be	-1.724153	1.374966	-0.242366
Be	-2.149983	-0.490720	-0.242366
Be	-0.956833	-1.986883	-0.242366
Be	0.956833	-1.986883	-0.242366
Be	1.724153	1.374966	-0.242366
Be	2.149983	-0.490720	-0.242366
H	1.324366	2.750073	-0.622944
H	-1.324366	2.750073	-0.622944
H	-2.975822	0.679212	-0.622944
H	-2.386424	-1.903110	-0.622944
H	0.000000	-3.052351	-0.622944
H	2.975822	0.679212	-0.622944

H	2.386424	-1.903110	-0.622944
Pt	0.000000	0.000000	0.142908

$Zn©Be_7H_7^+$ (**8**)

Be	0.000000	2.242431	0.000000
Be	1.753204	1.398133	0.000000
Be	2.186209	-0.498988	0.000000
Be	0.972955	-2.020361	0.000000
Be	-0.972955	-2.020361	0.000000
Be	-1.753204	1.398133	0.000000
Be	-2.186209	-0.498988	0.000000
H	-1.339626	2.781763	0.000000
H	1.339626	2.781763	0.000000
H	3.010113	0.687039	0.000000
H	2.413923	-1.925040	0.000000
H	0.000000	-3.087524	0.000000
H	-3.010113	0.687039	0.000000
H	-2.413923	-1.925040	0.000000
Zn	0.000000	0.000000	0.000000

$Cd©Be_7H_7^+$ (**9**)

Be	0.000000	2.312283	-0.136724
Be	1.807815	1.441685	-0.136724
Be	2.254309	-0.514531	-0.136724
Be	1.003262	-2.083295	-0.136724
Be	-1.003262	-2.083295	-0.136724
Be	-1.807815	1.441685	-0.136724
Be	-2.254309	-0.514531	-0.136724
H	-1.355232	2.814168	-0.316377
H	1.355232	2.814168	-0.316377
H	3.045179	0.695042	-0.316377
H	2.442044	-1.947465	-0.316377
H	0.000000	-3.123491	-0.316377
H	-3.045179	0.695042	-0.316377
H	-2.442044	-1.947465	-0.316377
Cd	0.000000	0.000000	0.125894

$Hg©Be_7H_7^+$ (**10**)

Be	0.000000	2.302200	0.000000
Be	1.799932	1.435398	0.000000
Be	2.244479	-0.512288	0.000000

Be	0.998887	-2.074210	0.000000
Be	-0.998887	-2.074210	0.000000
Be	-1.799932	1.435398	0.000000
Be	-2.244479	-0.512288	0.000000
H	-1.359673	2.823391	0.000000
H	1.359673	2.823391	0.000000
H	3.055158	0.697320	0.000000
H	2.450047	-1.953847	0.000000
H	0.000000	-3.133727	0.000000
H	-3.055158	0.697320	0.000000
H	-2.450047	-1.953847	0.000000
Hg	0.000000	0.000000	0.000000

b. B3LYP/BSI-optimized structures of molecules shown in Fig. 1.

B©$Be_6H_6^+$ (**1**)

H	2.73087200	0.00000000	0.00000000
H	1.36543600	2.36500500	0.00000000
H	-1.36543600	2.36500500	0.00000000
H	-2.73087200	0.00000000	0.00000000
H	-1.36543600	-2.36500500	0.00000000
H	1.36543600	-2.36500500	0.00000000
Be	0.00000000	1.88710100	0.00000000
Be	1.63427700	0.94355000	0.00000000
Be	-1.63427700	0.94355000	0.00000000
Be	-1.63427700	-0.94355000	0.00000000
Be	0.00000000	-1.88710100	0.00000000
Be	1.63427700	-0.94355000	0.00000000
B	0.00000000	0.00000000	0.00000000

Cu©Be_7H_7 (**2**)

Be	0.00000000	2.19039700	0.00000000
Be	1.71252200	1.36569000	0.00000000
Be	2.13548000	-0.48740900	0.00000000
Be	0.95037800	-1.97348000	0.00000000
Be	-0.95037800	-1.97348000	0.00000000
Be	-1.71252200	1.36569000	0.00000000
Be	-2.13548000	-0.48740900	0.00000000
H	-1.33925100	2.78098400	0.00000000
H	1.33925100	2.78098400	0.00000000

H	3.00927100	0.68684600	0.00000000
H	2.41324800	-1.92450100	0.00000000
H	0.00000000	-3.08666000	0.00000000
H	-3.00927100	0.68684600	0.00000000
H	-2.41324800	-1.92450100	0.00000000
Cu	0.00000000	0.00000000	0.00000000

Ag©Be_7H_7 (**3**)

Be	0.00000000	2.25440900	0.14366100
Be	-1.76256800	1.40560100	0.14366100
Be	-2.19788600	-0.50165300	0.14366100
Be	-0.97815100	-2.03115200	0.14366100
Be	0.97815100	-2.03115200	0.14366100
Be	1.76256800	1.40560100	0.14366100
Be	2.19788600	-0.50165300	0.14366100
H	1.34505800	2.79304100	0.40673200
H	-1.34505800	2.79304100	0.40673200
H	-3.02231700	0.68982400	0.40673200
H	-2.42371000	-1.93284400	0.40673200
H	0.00000000	-3.10004200	0.40673200
H	3.02231700	0.68982400	0.40673200
H	2.42371000	-1.93284400	0.40673200
Ag	0.00000000	0.00000000	-0.14616200

Au©Be_7H_7 (**4**)

Be	0.00000000	2.25317600	0.00000000
Be	1.76160400	1.40483200	0.00000000
Be	2.19668400	-0.50137900	0.00000000
Be	0.97761600	-2.03004100	0.00000000
Be	-0.97761600	-2.03004100	0.00000000
Be	-1.76160400	1.40483200	0.00000000
Be	-2.19668400	-0.50137900	0.00000000
H	-1.36123500	2.82663300	0.00000000
H	1.36123500	2.82663300	0.00000000
H	3.05866700	0.69812100	0.00000000
H	2.45286000	-1.95609100	0.00000000
H	0.00000000	-3.13732600	0.00000000
H	-3.05866700	0.69812100	0.00000000
H	-2.45286000	-1.95609100	0.00000000
Au	0.00000000	0.00000000	0.00000000

Ni©$Be_7H_7^-$ (**5**)

Be	0.00000000	2.16348400	-0.04007900
Be	1.69148000	1.34891000	-0.04007900
Be	2.10924100	-0.48142100	-0.04007900
Be	0.93870100	-1.94923200	-0.04007900
Be	-0.93870100	-1.94923200	-0.04007900
Be	-1.69148000	1.34891000	-0.04007900
Be	-2.10924100	-0.48142100	-0.04007900
H	-1.34181600	2.78630900	-0.17192800
H	1.34181600	2.78630900	-0.17192800
H	3.01503200	0.68816100	-0.17192800
H	2.41786800	-1.92818500	-0.17192800
H	0.00000000	-3.09256900	-0.17192800
H	-3.01503200	0.68816100	-0.17192800
H	-2.41786800	-1.92818500	-0.17192800
Ni	0.00000000	0.00000000	0.08306100

Pd©$Be_7H_7^-$ (**6**)

Be	0.00000000	2.20502400	-0.22743286
Be	-1.72395718	1.37480998	-0.22743286
Be	-2.14973944	-0.49066400	-0.22743286
Be	-0.95672406	-1.98665798	-0.22743286
Be	0.95672406	-1.98665798	-0.22743286
Be	1.72395718	1.37480998	-0.22743286
Be	2.14973944	-0.49066400	-0.22743286
H	1.30855870	2.71725014	-0.69317886
H	-1.30855870	2.71725014	-0.69317886
H	-2.94030471	0.67110536	-0.69317886
H	-2.35794130	-1.88039544	-0.69317886
H	0.00000000	-3.01592013	-0.69317886
H	2.94030471	0.67110536	-0.69317886
H	2.35794130	-1.88039544	-0.69317886
Pd	0.00000000	-0.00000000	0.24392114

Pt©$Be_7H_7^-$ (**7**)

Be	0.00000000	2.20826601	-0.23171299
Be	-1.72649189	1.37683134	-0.23171299
Be	-2.15290018	-0.49138542	-0.23171299
Be	-0.95813072	-1.98957893	-0.23171299
Be	0.95813072	-1.98957893	-0.23171299
Be	1.72649189	1.37683134	-0.23171299

Be	2.15290018	-0.49138542	-0.23171299
H	1.32989775	2.76156113	-0.59901800
H	-1.32989775	2.76156113	-0.59901800
H	-2.98825312	0.68204927	-0.59901800
H	-2.39639294	-1.91105960	-0.59901800
H	0.00000000	-3.06510161	-0.59901800
H	2.98825312	0.68204927	-0.59901800
H	2.39639294	-1.91105960	-0.59901800
Pt	-0.00000000	0.00000000	0.13693704

$Zn©Be_7H_7^+$ (**8**)

Be	0.00000000	2.24786700	0.00000000
Be	1.75745300	1.40152200	0.00000000
Be	2.19150800	-0.50019700	0.00000000
Be	0.97531300	-2.02525800	0.00000000
Be	-0.97531300	-2.02525800	0.00000000
Be	-1.75745300	1.40152200	0.00000000
Be	-2.19150800	-0.50019700	0.00000000
H	-1.34190400	2.78649300	0.00000000
H	1.34190400	2.78649300	0.00000000
H	3.01523100	0.68820700	0.00000000
H	2.41802800	-1.92831300	0.00000000
H	0.00000000	-3.09277400	0.00000000
H	-3.01523100	0.68820700	0.00000000
H	-2.41802800	-1.92831300	0.00000000
Zn	0.00000000	0.00000000	0.00000000

$Cd©Be_7H_7^+$ (**9**)

Be	0.00000000	2.31542400	-0.13669371
Be	1.81027138	1.44364325	-0.13669371
Be	2.25737149	-0.51523031	-0.13669371
Be	1.00462482	-2.08612494	-0.13669371
Be	-1.00462482	-2.08612494	-0.13669371
Be	-1.81027138	1.44364325	-0.13669371
Be	-2.25737149	-0.51523031	-0.13669371
H	-1.35734463	2.81855518	-0.31191971
H	1.35734463	2.81855518	-0.31191971
H	3.04992571	0.69612564	-0.31191971
H	2.44585052	-1.95050070	-0.31191971
H	0.00000000	-3.12836023	-0.31191971
H	-3.04992571	0.69612564	-0.31191971

H	-2.44585052	-1.95050070	-0.31191971
Cd	-0.00000000	0.00000000	0.12522629

$Hg©Be_7H_7^+$ (**10**)

Be	0.00000000	2.30731900	0.00000000
Be	-1.80393400	1.43859000	0.00000000
Be	-2.24946900	-0.51342700	0.00000000
Be	-1.00110800	-2.07882200	0.00000000
Be	1.00110800	-2.07882200	0.00000000
Be	1.80393400	1.43859000	0.00000000
Be	2.24946900	-0.51342700	0.00000000
H	1.36231600	2.82887900	0.00000000
H	-1.36231600	2.82887900	0.00000000
H	-3.06109700	0.69867500	0.00000000
H	-2.45480900	-1.95764500	0.00000000
H	0.00000000	-3.13981900	0.00000000
H	3.06109700	0.69867500	0.00000000
H	2.45480900	-1.95764500	0.00000000
Hg	0.00000000	0.00000000	0.00000000

c. B3LYP/BSI-optimized structures of molecules shown in Fig. S1.

$B©Be_5H_5$

Be	0.00000000	1.62539700	-0.02989800
Be	1.54584400	0.50227500	-0.02989800
Be	-1.54584400	0.50227500	-0.02989800
Be	-0.95538400	-1.31497400	-0.02989800
Be	0.95538400	-1.31497400	-0.02989800
H	1.35138900	1.86002700	-0.59628400
H	-1.35138900	1.86002700	-0.59628400
H	-2.18659300	-0.71046700	-0.59628400
H	0.00000000	-2.29912000	-0.59628400
H	2.18659300	-0.71046700	-0.59628400
B	0.00000000	0.00000000	0.71587700

$C©Be_5H_5^+$

C	0.00000000	0.00000000	0.24889100
Be	0.00000000	1.64547200	-0.01557900
Be	1.56493700	0.50847900	-0.01557900
Be	-1.56493700	0.50847900	-0.01557900

Be	-0.96718400	-1.33121500	-0.01557900
Be	0.96718400	-1.33121500	-0.01557900
H	1.42929800	1.96726000	-0.23635200
H	-1.42929800	1.96726000	-0.23635200
H	-2.31265300	-0.75142600	-0.23635200
H	0.00000000	-2.43166700	-0.23635200
H	2.31265300	-0.75142600	-0.23635200

N©Be_5H_5

Be	0.00000000	1.57621200	-0.07280400
Be	1.49906669	0.48707629	-0.07280400
Be	-1.49906669	0.48707629	-0.07280400
Be	-0.92647417	-1.27518229	-0.07280400
Be	0.92647417	-1.27518229	-0.07280400
H	1.26272131	1.73798678	-0.72100500
H	-1.26272131	1.73798678	-0.72100500
H	-2.04312599	-0.66385188	-0.72100500
H	0.00000000	-2.14826980	-0.72100500
H	2.04312599	-0.66385188	-0.72100500
N	0.00000000	-0.00000000	0.72301500

B©$Be_6H_6^+$

F	2.39816900	1.38936700	-0.25700081
F	0.00000000	2.76334500	0.47814219
F	-2.39816900	1.38936700	-0.25700081
F	-2.39816900	-1.38936700	-0.25700081
F	0.00000000	-2.76334500	0.47814219
F	2.39816900	-1.38936700	-0.25700081
Be	1.79733100	-0.00000000	-0.57305481
Be	0.98648600	1.59192100	0.31265419
Be	-0.98648600	1.59192100	0.31265419
Be	-1.79733100	-0.00000000	-0.57305481
Be	-0.98648600	-1.59192100	0.31265419
Be	0.98648600	-1.59192100	0.31265419
B	0.00000000	0.00000000	0.04548819

Be©Be_6H_6

H	-2.63550600	0.00000000	-0.50717100
H	-1.31781500	2.28205900	-0.50768300
H	1.31781500	2.28205900	-0.50768300
H	2.63550600	0.00000000	-0.50717100

H	1.31781500	-2.28205900	-0.50768300
H	-1.31781500	-2.28205900	-0.50768300
Be	0.00000000	1.90580200	0.00156400
Be	-1.65045800	0.95294400	0.00223100
Be	1.65045800	0.95294400	0.00223100
Be	1.65045800	-0.95294400	0.00223100
Be	0.00000000	-1.90580200	0.00156400
Be	-1.65045800	-0.95294400	0.00223100
Be	0.00000000	0.00000000	0.74921600

$B©Be_6H_6^+$

H	2.73087200	0.00000000	0.00000000
H	1.36543600	2.36500500	0.00000000
H	-1.36543600	2.36500500	0.00000000
H	-2.73087200	0.00000000	0.00000000
H	-1.36543600	-2.36500500	0.00000000
H	1.36543600	-2.36500500	0.00000000
Be	0.00000000	1.88710100	0.00000000
Be	1.63427700	0.94355000	0.00000000
Be	-1.63427700	0.94355000	0.00000000
Be	-1.63427700	-0.94355000	0.00000000
Be	0.00000000	-1.88710100	0.00000000
Be	1.63427700	-0.94355000	0.00000000
B	0.00000000	0.00000000	0.00000000

$Li©Be_7H_7$

Be	-1.45661400	1.88143600	0.10495200
Be	0.23649800	1.21405900	-0.42530500
Be	2.06656400	0.94986600	0.17789500
Be	2.09537200	-0.92050400	0.19137200
Be	0.26948600	-1.19773400	-0.42000400
Be	-1.79213000	-0.01917700	0.12964400
Be	-1.41200900	-1.90963300	0.09440300
H	-2.65268600	1.18706100	-0.18761300
H	-0.69315100	2.28084400	-1.00573500
H	1.57935700	1.83792300	-0.76777800
H	3.15595900	0.02915200	-0.12074800
H	1.62333700	-1.80717500	-0.76196100
H	-2.62411800	-1.24407900	-0.19785600
H	-0.63248400	-2.28967000	-1.00957600
Li	0.07170400	0.00423100	1.54648100

$Na©Be_7H_7$

Be	2.64461300	-1.11202300	0.04600800
Be	0.75583700	-1.47787600	-0.41540400
Be	-1.32212400	-1.55871000	-0.46096500
Be	-2.76723800	-0.32424100	-0.51125800
Be	-0.62988200	0.29748300	-0.91277800
Be	1.31179000	0.52307400	-0.70233300
Be	0.53151000	2.22341400	-1.17034300
H	3.91260600	-0.93856100	0.41864700
H	1.87706400	-2.33098900	-0.12730400
H	-0.29142700	-2.40592700	-0.07909200
H	-2.69695800	-1.83396400	-0.30451100
H	-3.85483900	0.44945100	-0.51115600
H	1.96948200	1.74859500	-0.93206400
H	0.15520400	3.48100600	-1.42924900
Na	-0.28810500	0.68599100	1.77027400

$Be©Be_7H_7^+$

Be	1.14324300	1.83136400	0.05607900
Be	2.13847000	0.22886400	0.27114200
Be	1.53728000	-1.51005100	-0.18892700
Be	-0.25435100	-2.14001000	-0.17985300
Be	-1.81462000	-1.15806500	0.26467700
Be	-0.71307000	2.03172600	-0.28195800
Be	-2.03689700	0.71600300	0.05859300
H	0.34350200	2.99765700	-0.18955700
H	2.54288600	1.60521000	0.27723100
H	2.85284500	-0.99918600	0.07049400
H	0.99504600	-2.83275300	-0.31063700
H	-1.60193100	-2.56389300	0.07274900
H	-2.14128100	2.12634000	-0.18718200
H	-2.98969100	-0.33525900	0.27388400
Be	-0.00040000	0.00063900	-0.00149800

$Mg©Be_7H_7^+$

Be	0.00000000	2.36443900	0.00000000
Be	-1.84859300	1.47420300	0.00000000
Be	-2.30515700	-0.52613700	0.00000000
Be	-1.02589200	-2.13028600	0.00000000
Be	1.02589200	-2.13028600	0.00000000

Be	1.84859300	1.47420300	0.00000000
Be	2.30515700	-0.52613700	0.00000000
H	1.38097500	2.86762300	0.00000000
H	-1.38097500	2.86762300	0.00000000
H	-3.10302200	0.70824400	0.00000000
H	-2.48843000	-1.98445700	0.00000000
H	0.00000000	-3.18282200	0.00000000
H	3.10302200	0.70824400	0.00000000
H	2.48843000	-1.98445700	0.00000000
Mg	0.00000000	0.00000000	0.00000000

d. B3LYP/BSI-optimized structures of molecules shown in Fig. S4.

Co©$Be_8H_8^-$

Be	-1.47671663	1.54069946	0.02470784
Be	1.47671663	-1.54069946	0.02470784
Be	-1.47111114	-1.54557272	0.02624184
Be	1.47111114	1.54557272	0.02624184
Be	-0.00242960	1.77178400	-1.11701416
Be	0.00242960	-1.77178400	-1.11701416
Be	-1.88596316	-0.00277743	1.01778284
Be	1.88596316	0.00277743	1.01778284
H	-2.65127057	1.26886701	0.87801784
H	-2.64619851	-1.27756975	0.88020084
H	-1.24696301	-2.59233390	-0.98427516
H	1.25491163	-2.58743511	-0.98647616
H	-1.25491163	2.58743511	-0.98647616
H	1.24696301	2.59233390	-0.98427516
H	2.64619851	1.27756975	0.88020084
H	2.65127057	-1.26886701	0.87801784
Co	0.00000000	-0.00000000	0.03004884

Rh©$Be_8H_8^-$

Be	2.03841900	0.00000000	0.89743300
Be	-2.03841900	0.00000000	0.89743300
Be	0.00000000	-2.03841900	-0.89743300
Be	0.00000000	2.03841900	-0.89743300
Be	1.60863700	1.60863700	0.00000000
Be	-1.60863700	-1.60863700	0.00000000
Be	1.60863700	-1.60863700	0.00000000

Be	-1.60863700	1.60863700	0.00000000
H	2.81095600	-1.27380100	0.77020900
H	1.27380100	-2.81095600	-0.77020900
H	-1.27380100	-2.81095600	-0.77020900
H	-2.81095600	-1.27380100	0.77020900
H	2.81095600	1.27380100	0.77020900
H	1.27380100	2.81095600	-0.77020900
H	-1.27380100	2.81095600	-0.77020900
H	-2.81095600	1.27380100	0.77020900
Rh	0.00000000	0.00000000	0.00000000

$Ir©Be_8H_8^-$

Be	2.04255000	0.00000000	0.89674400
Be	-2.04255000	0.00000000	0.89674400
Be	0.00000000	-2.04255000	-0.89674400
Be	0.00000000	2.04255000	-0.89674400
Be	1.61168900	1.61168900	0.00000000
Be	-1.61168900	-1.61168900	0.00000000
Be	1.61168900	-1.61168900	0.00000000
Be	-1.61168900	1.61168900	0.00000000
H	2.82237300	-1.27024500	0.75379900
H	1.27024500	-2.82237300	-0.75379900
H	-1.27024500	-2.82237300	-0.75379900
H	-2.82237300	-1.27024500	0.75379900
H	2.82237300	1.27024500	0.75379900
H	1.27024500	2.82237300	-0.75379900
H	-1.27024500	2.82237300	-0.75379900
H	-2.82237300	1.27024500	0.75379900
Ir	0.00000000	0.00000000	0.00000000

$Ni©Be_8H_8$

Be	-0.47964004	0.64796361	1.96790780
Be	-0.88003918	-1.15362400	-1.47479448
Be	0.40482208	1.97968622	-0.94264051
Be	0.86102677	-1.65463424	0.96961089
Be	-0.88003918	-1.15362400	1.47479448
Be	-0.47964004	0.64796361	-1.96790780
Be	0.40482208	1.97968622	0.94264051
Be	0.86102677	-1.65463424	-0.96961089
H	-0.09067093	2.02652013	2.32204555
H	0.76010216	3.04397599	0.00000000

H	-0.09067093	2.02652013	-2.32204555
H	-1.32291311	-0.32487952	-2.61670443
H	-1.32291311	-0.32487952	2.61670443
H	-0.07476428	-2.31490032	1.88603206
H	1.54991771	-2.49584707	0.00000000
H	-0.07476428	-2.31490032	-1.88603206
Ni	0.05126492	0.07422805	0.00000000

Pd©Be_8H_8

Be	-2.08342096	-0.21402550	-0.86904361
Be	2.08342096	0.21402550	-0.86904361
Be	0.21562384	-2.08832095	0.85871328
Be	-0.21562384	2.08832095	0.85871328
Be	-1.80636039	1.41206022	0.06853639
Be	1.80636039	-1.41206022	0.06853639
Be	-1.42039768	-1.79916931	-0.05826166
Be	1.42039768	1.79916931	-0.05826166
H	-2.64056463	-1.56740908	-0.80632761
H	-0.95747137	-2.95039459	0.69363032
H	1.57085445	-2.64057353	0.80335723
H	2.95086175	-0.95485514	-0.69513680
H	-2.95086175	0.95485514	-0.69513680
H	-1.57085445	2.64057353	0.80335723
H	0.95747137	2.95039459	0.69363032
H	2.64056463	1.56740908	-0.80632761
Pd	-0.00000000	0.00000000	0.00020431

Pt©Be_8H_8

Be	2.22416818	-0.46236148	0.04606812
Be	-2.22416818	0.46236148	0.04606812
Be	0.50042037	2.22100231	-0.01865488
Be	-0.50042037	-2.22100231	-0.01865488
Be	1.12069540	-1.77353583	0.86305712
Be	-1.12069540	1.77353583	0.86305712
Be	1.74801916	1.10543790	-0.91480788
Be	-1.74801916	-1.10543790	-0.91480788
H	3.04478161	0.44203509	-0.74068088
H	1.66362097	2.56653390	-0.81841088
H	-0.45081764	3.07102893	0.66312012
H	-2.58477884	1.67997316	0.75069812
H	2.58477884	-1.67997316	0.75069812

H	0.45081764	-3.07102893	0.66312012
H	-1.66362097	-2.56653390	-0.81841088
H	-3.04478161	-0.44203509	-0.74068088
Pt	0.00000000	0.00000000	0.00622112

$Cu©Be_8H_8^+$

Be	-0.93829286	-1.17152234	1.48061400
Be	-0.35220999	0.60197783	-2.05301600
Be	0.80722381	-1.75107335	-0.99282500
Be	0.28671738	2.07332533	0.96471000
Be	-0.35220999	0.60197783	2.05301600
Be	-0.93829286	-1.17152234	-1.48061400
Be	0.80722381	-1.75107335	0.99282500
Be	0.28671738	2.07332533	-0.96471000
H	-0.18514967	-2.35383938	1.84945700
H	1.45087961	-2.56563215	0.00000000
H	-0.18514967	-2.35383938	-1.84945700
H	-1.30931858	-0.31745220	-2.59468000
H	-1.30931858	-0.31745220	2.59468000
H	-0.11855271	2.01678382	2.34402100
H	0.53890856	3.13432572	0.00000000
H	-0.11855271	2.01678382	-2.34402100
Cu	0.09685335	0.09374697	0.00000000

$Ag©Be_8H_8^+$

Be	0.96574905	2.10694558	0.51900500
Be	-0.96574905	-2.10694558	0.51900500
Be	-2.10694558	0.96574905	-0.51900500
Be	2.10694558	-0.96574905	-0.51900500
Be	2.10694558	0.96574905	-0.51900500
Be	-2.10694558	-0.96574905	-0.51900500
Be	-0.96574905	2.10694558	0.51900500
Be	0.96574905	-2.10694558	0.51900500
H	0.00000000	3.10985115	0.86566400
H	-2.29390851	2.29390851	-0.00000000
H	-3.10985115	0.00000000	-0.86566400
H	-2.29390851	-2.29390851	0.00000000
H	2.29390851	2.29390851	0.00000000
H	3.10985115	-0.00000000	-0.86566400
H	2.29390851	-2.29390851	-0.00000000
H	0.00000000	-3.10985115	0.86566400

Ag	0.00000000	0.00000000	0.00000000

$Au©Be_8H_8^+$

Be	0.96817700	2.03641700	0.59252000
Be	-0.96817700	-2.03641700	0.59252000
Be	2.03641700	-0.96817700	-0.59252000
Be	-2.03641700	0.96817700	-0.59252000
Be	-0.96817700	2.03641700	0.59252000
Be	0.96817700	-2.03641700	0.59252000
Be	2.03641700	0.96817700	-0.59252000
Be	-2.03641700	-0.96817700	-0.59252000
H	2.26212300	2.26212300	0.00000000
H	3.02710400	-0.00000000	-0.97691300
H	2.26212300	-2.26212300	-0.00000000
H	-0.00000000	-3.02710400	0.97691300
H	0.00000000	3.02710400	0.97691300
H	-2.26212300	2.26212300	-0.00000000
H	-3.02710400	-0.00000000	-0.97691300
H	-2.26212300	-2.26212300	0.00000000
Au	0.00000000	0.00000000	-0.00000000

e. B3LYP/BSI-optimized structures of molecules shown in Fig. S5.

1

H	2.73087200	0.00000000	0.00000000
H	1.36543600	2.36500500	0.00000000
H	-1.36543600	2.36500500	0.00000000
H	-2.73087200	0.00000000	0.00000000
H	-1.36543600	-2.36500500	0.00000000
H	1.36543600	-2.36500500	0.00000000
Be	0.00000000	1.88710100	0.00000000
Be	1.63427700	0.94355000	0.00000000
Be	-1.63427700	0.94355000	0.00000000
Be	-1.63427700	-0.94355000	0.00000000
Be	0.00000000	-1.88710100	0.00000000
Be	1.63427700	-0.94355000	0.00000000
B	0.00000000	0.00000000	0.00000000

1a

H	-0.67237991	1.13847844	2.05817500

H	-0.15658906	2.67315578	0.00000000
H	-0.67237991	1.13847844	-2.05817500
H	-1.28299642	-1.33252306	1.32953200
H	0.45576023	-2.57928711	0.00000000
H	-1.28299642	-1.33252306	-1.32953200
Be	0.16270932	1.61886941	-0.96051100
Be	-0.42764127	-0.17254588	-1.45311000
Be	-0.65329588	-1.54698323	0.00000000
Be	1.29264075	-1.44565737	0.00000000
Be	0.16270932	1.61886941	0.96051100
Be	-0.42764127	-0.17254588	1.45311000
B	0.63473154	0.13883895	0.00000000

1b

H	0.00000000	0.00000000	3.41773200
H	0.00000000	-2.30681000	-0.96944800
H	2.19390700	-0.71284400	-0.96944800
H	1.35590900	1.86624900	-0.96944800
H	-1.35590900	1.86624900	-0.96944800
H	-2.19390700	-0.71284400	-0.96944800
Be	0.00000000	1.66135600	-0.42637100
Be	-1.58004300	0.51338700	-0.42637100
Be	-0.97652100	-1.34406500	-0.42637100
Be	0.97652100	-1.34406500	-0.42637100
Be	1.58004300	0.51338700	-0.42637100
Be	0.00000000	0.00000000	2.10137600
B	0.00000000	0.00000000	0.31028400

1c

B	-0.72965700	0.51314300	0.00000000
Be	0.61198400	1.21495100	0.98878200
Be	0.61198400	-0.82259100	1.04454000
Be	-1.32967500	-0.45669700	1.26140400
Be	0.61198400	-0.82259100	-1.04454000
Be	0.61198400	1.21495100	-0.98878200
Be	-1.32967500	-0.45669700	-1.26140400
H	-0.48629500	-1.40073500	-1.89493700
H	-0.48629500	-1.40073500	1.89493700
H	1.37080100	0.23408100	1.73015800
H	1.44539000	1.88118600	0.00000000
H	1.37080100	0.23408100	-1.73015800

H	1.27954500	-1.59889800	0.00000000

1d

B	-0.25637700	-0.00464200	0.83886500
Be	1.69829400	0.02672100	-0.75841500
Be	1.44900500	-0.04530100	1.19400200
Be	0.35508900	-1.39795800	-0.36796100
Be	0.32736000	1.42605900	-0.31819200
Be	-1.58083000	0.96156600	-0.01309100
Be	-1.56101400	-0.98458900	-0.03510700
H	1.29016800	1.26623500	-1.35178500
H	-2.37343400	-0.01118800	-0.73916400
H	0.20162600	-0.02563500	1.98571600
H	1.26034200	-1.15360500	-1.43757300
H	-0.90612900	-2.04476000	-0.74861600
H	-0.94230500	2.04616900	-0.70784500

2

Be	0.00000000	2.19039700	0.00000000
Be	1.71252200	1.36569000	0.00000000
Be	2.13548000	-0.48740900	0.00000000
Be	0.95037800	-1.97348000	0.00000000
Be	-0.95037800	-1.97348000	0.00000000
Be	-1.71252200	1.36569000	0.00000000
Be	-2.13548000	-0.48740900	0.00000000
H	-1.33925100	2.78098400	0.00000000
H	1.33925100	2.78098400	0.00000000
H	3.00927100	0.68684600	0.00000000
H	2.41324800	-1.92450100	0.00000000
H	0.00000000	-3.08666000	0.00000000
H	-3.00927100	0.68684600	0.00000000
H	-2.41324800	-1.92450100	0.00000000
Cu	0.00000000	0.00000000	0.00000000

2a

H	-0.15229800	1.20301800	1.85818200
H	3.53750400	-0.64254200	-0.11152900
H	1.79350700	-2.54802100	0.34604200
H	0.43344700	-1.24282500	1.86429100
H	-1.88525500	1.44150300	0.14151500
H	0.33207100	2.82343000	0.10862400

H	2.73089900	1.89987900	0.01186100
Be	2.64073500	0.49351500	-0.35361200
Be	0.79990700	-0.04878500	-0.76637800
Be	0.52968000	0.09036900	1.26068500
Be	-0.51546900	1.66345000	0.47223200
Be	1.31432900	1.88115300	-0.35180400
Be	2.30545600	-1.37224100	-0.32222800
Be	0.59053700	-1.68344000	0.48161100
Cu	-1.29139900	-0.24243200	-0.20348300

2b

H	-3.48027500	-0.33848600	-0.12451400
H	-2.50376100	2.13844300	0.23783400
H	-0.53606100	-0.98402400	1.96111400
H	2.10832500	1.29879000	0.01651800
H	0.04480900	2.87267900	-0.25202100
H	-1.91188000	-2.41463100	0.40463800
H	-1.76443300	-0.96054300	-1.65693600
Be	-2.33605100	-1.23314800	-0.37899600
Be	-1.06762900	1.97457600	-0.05093000
Be	-0.80775200	-0.09463500	-0.88599700
Be	0.78568700	1.74374400	0.27591200
Be	-0.72571600	-1.59351400	0.67965600
Be	-0.55588400	0.25824600	1.08636100
Be	-2.50436400	0.73065200	-0.02516500
Cu	1.27207300	-0.30192800	-0.11689600

2c

Be	0.63013100	-0.30194000	-0.84673700
Be	0.15981500	-1.75327300	0.34676300
Be	0.88861900	0.25674400	1.04388400
Be	2.61882700	0.10659800	-0.22003500
Be	1.63008500	1.71833400	-0.31023800
Be	-0.29147900	1.73946900	0.27168000
Be	1.96906300	-1.71125800	-0.06522600
H	0.12536500	1.34744300	1.63466800
H	-1.68517000	1.62509000	0.03260300
H	0.70812500	2.79849500	-0.20245200
H	2.76899500	1.29744900	-1.10028500
H	1.21542900	-2.77989000	0.51495900
H	3.32327300	-1.15965600	-0.00093800

H	2.29754600	1.05821500	0.93238400
Cu	-1.35082100	-0.15192600	-0.09280300

2d

Be	-2.07552200	-1.22618600	0.83612900
Be	-1.31991900	1.99813300	-0.64537100
Be	0.20053300	1.51278600	0.40868400
Be	-1.80092600	-1.40155300	-1.07178200
Be	-0.38362800	-0.16908200	1.20350100
Be	-0.61695400	0.04125200	-0.90737800
Be	-2.39677300	0.45923500	-0.11710900
H	-1.10579300	-1.19563300	1.93808500
H	-3.07133200	-0.19968500	1.02984800
H	-2.65220900	1.92194600	-0.17484100
H	-0.34947500	2.83496000	0.05194800
H	-0.59236300	-1.22740200	-1.77923000
H	-2.21183400	-2.39540400	-0.08748300
H	-0.01238800	1.09672600	1.78866300
Cu	1.50235000	-0.19634000	-0.05495500

3

Be	0.00000000	2.25440900	0.14366100
Be	-1.76256800	1.40560100	0.14366100
Be	-2.19788600	-0.50165300	0.14366100
Be	-0.97815100	-2.03115200	0.14366100
Be	0.97815100	-2.03115200	0.14366100
Be	1.76256800	1.40560100	0.14366100
Be	2.19788600	-0.50165300	0.14366100
H	1.34505800	2.79304100	0.40673200
H	-1.34505800	2.79304100	0.40673200
H	-3.02231700	0.68982400	0.40673200
H	-2.42371000	-1.93284400	0.40673200
H	0.00000000	-3.10004200	0.40673200
H	3.02231700	0.68982400	0.40673200
H	2.42371000	-1.93284400	0.40673200
Ag	0.00000000	0.00000000	-0.14616200

3a

Be	-1.00818900	-0.51000600	0.23822700
Be	-1.96176800	1.96905700	-0.19367300

Be	-2.34344000	-1.66935200	-0.92894400
Be	-2.40374700	0.55896800	1.24760800
Be	-2.34906800	0.25757900	-1.04068300
Be	-3.09308400	-1.16105800	0.69259600
Be	-0.19445300	1.18210200	-0.57190900
H	-2.79162600	-0.79095600	-1.95220800
H	-0.63840900	2.56345500	-0.44467100
H	-3.49130900	-0.32932500	1.77918000
H	-2.51467800	2.01815300	1.15584500
H	-2.81923500	1.65332600	-1.28897000
H	-3.45979900	-2.26280200	-0.15169800
H	-1.18272400	-0.11267900	1.63568700
Ag	1.49601600	-0.11166700	0.03178600

3b

Be	0.43541400	0.86743800	-0.39209100
Be	1.99580900	-0.60856100	1.03203100
Be	0.38477600	-1.08888900	0.11816900
Be	2.02620200	-0.27289200	-0.85320800
Be	4.12199100	-0.95818200	-0.67308400
Be	2.15975600	1.60434900	-0.06303000
Be	3.63301600	0.45555300	0.66566400
H	4.70664300	-1.74087100	-1.58462600
H	3.41262900	1.93483400	0.55113400
H	1.68609700	1.00540200	-1.44521300
H	4.87672800	-0.08581100	0.26061600
H	0.85759700	2.21274900	0.06564800
H	3.11970800	-0.22506900	1.85346300
H	0.84202300	-1.39351200	1.45518000
Ag	-1.67083600	-0.03623400	-0.01051100

3c

Be	-0.49030000	-1.44317100	-0.67941400
Be	-1.84993900	1.00864700	1.06650100
Be	-0.35888200	1.63512200	-0.46793800
Be	-0.83628600	-0.77837300	1.15270400
Be	-1.73589700	0.16847000	-1.30691700
Be	-2.30199500	-1.56419400	-0.10055800
Be	-3.34843700	0.15188100	-0.02639200
H	-3.69104700	-1.22973700	0.14493000
H	-1.05138800	1.36671300	-1.70750700

H	-3.15746300	0.59816100	-1.35584500
H	-3.31023800	1.09637700	1.06214600
H	-1.24212900	0.23888300	2.12470000
H	-1.15877500	2.17229800	0.64415800
H	0.97772500	2.02410600	-0.48976000
Ag	1.19830300	-0.06341100	0.02181300

3d

Be	-0.96707100	-0.55565700	-0.90437400
Be	-0.57779800	-1.37844700	1.16014600
Be	-1.00315600	0.49438700	0.93058700
Be	-1.08152000	2.65959200	0.46366100
Be	-1.93115400	-2.07779900	-0.07182200
Be	-2.08596100	1.36207600	-0.65236900
Be	-2.88425900	-0.30857600	-0.27370300
H	-3.32772300	-1.67112000	-0.04342500
H	-1.28604600	-1.95803000	-1.33176900
H	-1.24696700	-2.66870400	1.10779700
H	-3.48129600	0.95820100	-0.25394300
H	-0.41043800	3.69838300	0.98022900
H	-1.87569500	2.75086000	-0.80353400
H	-0.73481600	-0.37412100	2.15045500
Ag	1.15929000	-0.03229300	-0.09392200

4

Be	0.00000000	2.25317600	0.00000000
Be	1.76160400	1.40483200	0.00000000
Be	2.19668400	-0.50137900	0.00000000
Be	0.97761600	-2.03004100	0.00000000
Be	-0.97761600	-2.03004100	0.00000000
Be	-1.76160400	1.40483200	0.00000000
Be	-2.19668400	-0.50137900	0.00000000
H	-1.36123500	2.82663300	0.00000000
H	1.36123500	2.82663300	0.00000000
H	3.05866700	0.69812100	0.00000000
H	2.45286000	-1.95609100	0.00000000
H	0.00000000	-3.13732600	0.00000000
H	-3.05866700	0.69812100	0.00000000
H	-2.45286000	-1.95609100	0.00000000
Au	0.00000000	0.00000000	0.00000000

4a

Be	-2.77236800	-1.28276000	0.84252300
Be	-2.15867300	1.97563500	-0.64527800
Be	-0.60170600	1.57602300	0.41746300
Be	-2.54024400	-1.42599300	-1.07664400
Be	-1.09953400	-0.17330600	1.19739500
Be	-1.39921400	0.05911900	-0.95349600
Be	-3.18435400	0.38439700	-0.10614500
H	-1.77549600	-1.23290500	1.92238900
H	-3.79910200	-0.29700700	1.07141900
H	-3.44665100	1.84222000	-0.07455700
H	-1.22685900	2.85926900	0.06214800
H	-1.34911100	-1.21166500	-1.80067000
H	-2.87927600	-2.44150400	-0.08596500
H	-0.86491300	1.13067800	1.78838600
Au	0.89070600	-0.06457700	-0.02008100

4b

Be	-1.33195300	-0.50932700	0.26230900
Be	-2.31246100	1.97771400	-0.18873800
Be	-2.64571700	-1.67150200	-0.93420600
Be	-2.75546500	0.55612800	1.24359200
Be	-2.65409800	0.25705300	-1.04688600
Be	-3.42146100	-1.17122900	0.67681500
Be	-0.55063100	1.20663100	-0.59386000
H	-3.08885700	-0.79244500	-1.95915600
H	-0.99850400	2.59088200	-0.43503600
H	-3.85261800	-0.33596000	1.74724900
H	-2.87524700	2.01604800	1.15544600
H	-3.14376400	1.65086100	-1.29998700
H	-3.77418900	-2.26958300	-0.17742100
H	-1.54877600	-0.11189400	1.65978100
Au	1.03758400	-0.06746500	0.02067100

4c

H	-1.74280000	-0.58264900	-1.52981400
H	-3.64603600	-2.30241300	0.13366300
H	-3.37878200	-0.64283100	1.94747100
H	-0.97075100	2.61537100	0.32629500
H	-2.79061000	1.95249400	-1.33415400
H	-3.17504800	1.74999600	1.11277900

H	-3.84967300	-0.39451500	-1.68073500
Be	-2.77360300	0.50555600	-1.27113100
Be	-3.14699800	-1.26786800	-0.77064200
Be	-2.76814700	-1.55454900	1.04925500
Be	-0.52259700	1.24893900	0.58814600
Be	-2.25325500	1.95709400	0.03947800
Be	-1.35713100	-0.46716900	-0.09109900
Be	-2.70756500	0.34648900	1.06789600
Au	1.03380900	-0.06923300	-0.01801400

4d

H	-3.40852700	2.03845200	-0.93064800
H	-5.45854000	-1.46058700	1.23882500
H	-4.07306600	-1.72564800	-0.74943900
H	-5.22150300	0.43592600	-0.34693000
H	-0.88965100	2.34845000	-0.36904700
H	-1.61464000	-1.54337100	-1.23911500
H	-1.99524800	-1.18424300	0.78980500
Be	-3.95477700	0.97652700	-0.13490400
Be	-2.37491700	0.19963400	0.92948000
Be	-0.97014700	-0.63159100	-0.30541900
Be	-2.83147200	-1.11114300	-0.55990800
Be	-2.14544500	1.63422900	-0.38373500
Be	-0.54755000	1.23508800	0.49925700
Be	-4.74820700	-0.84600400	0.28428500
Au	1.17659800	-0.05994900	0.00367500

f. B3LYP/BSI-optimized structures of molecules shown in Fig. S6.

5

Be	0.00000000	2.16348400	-0.04007900
Be	1.69148000	1.34891000	-0.04007900
Be	2.10924100	-0.48142100	-0.04007900
Be	0.93870100	-1.94923200	-0.04007900
Be	-0.93870100	-1.94923200	-0.04007900
Be	-1.69148000	1.34891000	-0.04007900
Be	-2.10924100	-0.48142100	-0.04007900
H	-1.34181600	2.78630900	-0.17192800
H	1.34181600	2.78630900	-0.17192800
H	3.01503200	0.68816100	-0.17192800
H	2.41786800	-1.92818500	-0.17192800

H	0.00000000	-3.09256900	-0.17192800
H	-3.01503200	0.68816100	-0.17192800
H	-2.41786800	-1.92818500	-0.17192800
Ni	0.00000000	0.00000000	0.08306100

5a

Be	0.00000000	0.00000000	2.06856100
Be	0.00000000	1.95582300	0.55107900
Be	-1.69379200	-0.97791100	0.55107900
Be	0.00000000	-1.51382200	-1.29384800
Be	1.31100800	0.75691100	-1.29384800
Be	1.69379200	-0.97791100	0.55107900
Be	-1.31100800	0.75691100	-1.29384800
H	0.00000000	0.00000000	3.42282500
H	0.00000000	3.25723700	0.92500100
H	2.19495300	1.26725700	-2.18343800
H	-2.82085000	-1.62861900	0.92500100
H	0.00000000	-2.53451400	-2.18343800
H	2.82085000	-1.62861900	0.92500100
H	-2.19495300	1.26725700	-2.18343800
Ni	0.00000000	0.00000000	0.03541000

5b

Be	0.98875800	1.82432300	0.00000000
Be	-1.61182700	-1.00078400	0.00000000
Be	0.02898700	0.12350100	1.98453800
Be	0.02898700	0.12350100	-1.98453800
Be	0.02898700	-2.16169600	0.00000000
Be	-1.53868900	1.38528400	0.00000000
Be	1.85928100	-0.55775600	0.00000000
H	1.66021700	3.00256400	0.00000000
H	-1.62776700	-2.40528800	0.00000000
H	0.65332100	-3.36432700	0.00000000
H	0.05922500	0.16344900	3.33854500
H	0.05922500	0.16344900	-3.33854500
H	-2.49251000	2.35281200	0.00000000
H	3.17800200	-0.86492000	0.00000000
Ni	-0.02241600	0.07167000	0.00000000

5c

Be	-1.43969900	-1.65100500	-0.15934300

Be	-2.11927000	0.53091800	-0.15776400
Be	-0.74041100	1.93487700	0.04336000
Be	1.15103100	1.69716300	0.07350500
Be	2.23256300	0.03839000	-0.33922800
Be	0.95613800	-1.89828200	0.34517200
Be	-0.16725900	0.31021600	1.56354900
H	-2.16964200	-2.79210800	-0.25948100
H	-3.34216100	-0.06074700	-0.27522300
H	-2.14103800	2.08321600	-0.10227300
H	0.33470300	2.93658800	0.02370100
H	2.53451500	1.58776700	-0.13234100
H	1.50683600	-3.07771300	0.73679500
H	3.39275600	-0.61346500	-0.62677300
Ni	0.01398800	-0.13973700	-0.17290700

5d

Be	-0.00800700	2.28546500	0.03353500
Be	-1.67143100	0.61254600	-0.10666500
Be	-3.22216400	-0.67088600	-0.11707800
Be	0.77399500	-1.84243100	0.01225300
Be	-1.10587100	-1.32308700	-0.20673400
Be	2.44711800	-0.72378400	-0.01981600
Be	-0.31484400	-0.19368200	1.47743100
H	-4.47214400	-1.20083700	-0.14813100
H	-0.25728700	3.61780400	0.12896700
H	3.78143800	-0.48593800	-0.02835900
H	2.10695100	-2.29671900	0.00695100
H	-0.41501800	-2.64192400	-0.17831300
H	-3.08501400	0.85491300	-0.09409700
H	1.35668100	1.60833500	-0.13347900
Ni	0.47818600	0.28456400	-0.13733000

6

Be	0.00000000	2.20502400	-0.22743286
Be	-1.72395718	1.37480998	-0.22743286
Be	-2.14973944	-0.49066400	-0.22743286
Be	-0.95672406	-1.98665798	-0.22743286
Be	0.95672406	-1.98665798	-0.22743286
Be	1.72395718	1.37480998	-0.22743286
Be	2.14973944	-0.49066400	-0.22743286

H	1.30855870	2.71725014	-0.69317886
H	-1.30855870	2.71725014	-0.69317886
H	-2.94030471	0.67110536	-0.69317886
H	-2.35794130	-1.88039544	-0.69317886
H	0.00000000	-3.01592013	-0.69317886
H	2.94030471	0.67110536	-0.69317886
H	2.35794130	-1.88039544	-0.69317886
Pd	0.00000000	-0.00000000	0.24392114

6a

H	-3.75801800	-0.91245300	0.51227600
H	0.39661700	2.44464100	0.72232400
H	-2.57942300	-2.98020300	0.97465700
H	2.07246100	1.33343800	2.13243500
H	-1.14372200	2.55748900	-1.10002600
H	-0.31585500	0.72637200	2.27414600
H	-3.39609100	1.46396600	-0.42962300
Be	-2.44098800	-1.69709200	0.55261000
Be	0.86286300	1.23766300	1.50402100
Be	-2.06596500	1.48060200	-0.95130300
Be	-0.88944100	0.06772000	1.13165000
Be	-1.14824500	-0.34704900	-0.72668000
Be	-0.20935900	1.64320300	-0.30061700
Be	-2.93386800	0.11192800	-0.00083400
Pd	0.95704400	-0.31785100	-0.21568700

6b

Be	-0.00000000	-0.00000000	2.17982596
Be	0.00000000	2.07725549	0.57799037
Be	-1.79895603	-1.03862775	0.57799037
Be	0.00000000	-1.61875701	-1.37778979
Be	1.40188469	0.80937850	-1.37778979
Be	1.79895603	-1.03862775	0.57799037
Be	-1.40188469	0.80937850	-1.37778979
H	0.00000000	-0.00000000	3.53098096
H	0.00000000	3.38191776	0.92721137
H	2.27916641	1.31587734	-2.26940705
H	-2.92882669	-1.69095888	0.92721137
H	0.00000000	-2.63175468	-2.26940705
H	2.92882669	-1.69095888	0.92721137
H	-2.27916641	1.31587734	-2.26940705

Pd	0.00000000	-0.00000000	0.02986696

6c

Be	0.93687300	0.17032600	-0.92174800
Be	0.97579000	-0.03783100	0.99543400
Be	0.14703600	2.09670500	-0.06233100
Be	2.86769500	-0.00866100	-0.29625200
Be	2.07572900	1.69055400	-0.19677400
Be	0.09641300	-1.99310200	-0.51216500
Be	1.96822000	-1.64392100	0.39739200
H	1.44322300	2.91551800	0.05179800
H	3.48274500	1.29221300	-0.10599800
H	-0.96815400	2.88502300	0.04846700
H	3.39348500	-1.32239200	0.07012300
H	1.30514400	-2.81391300	-0.00844900
H	-0.77162200	-2.87091800	-1.10391500
H	1.54474500	-1.21906600	1.72580100
Pd	-0.99349100	0.00081000	0.03712900

6d

H	4.24033600	-0.00100300	-0.06105400
H	2.34950400	-1.26709700	-1.00543500
H	-1.42653600	1.41306800	1.85129400
H	0.38075200	2.54307200	0.14631700
H	0.38117700	-2.53668200	0.23472200
H	2.34910400	1.23089000	-1.04940600
H	-1.42667300	-1.34739200	1.89934200
Be	1.14825400	0.02466000	1.41676400
Be	1.29993300	1.33401100	-0.11851700
Be	-0.11971400	-1.59682400	1.21791600
Be	-0.11886500	1.63830900	1.16250400
Be	-0.86448900	0.03286400	1.88118200
Be	2.87305100	-0.00332100	-0.18940500
Be	1.29997900	-1.33757700	-0.07186500
Pd	-0.62870100	-0.00876800	-0.50456700

7

Be	0.00000000	2.20826601	-0.23171299
Be	-1.72649189	1.37683134	-0.23171299
Be	-2.15290018	-0.49138542	-0.23171299

Be	-0.95813072	-1.98957893	-0.23171299
Be	0.95813072	-1.98957893	-0.23171299
Be	1.72649189	1.37683134	-0.23171299
Be	2.15290018	-0.49138542	-0.23171299
H	1.32989775	2.76156113	-0.59901800
H	-1.32989775	2.76156113	-0.59901800
H	-2.98825312	0.68204927	-0.59901800
H	-2.39639294	-1.91105960	-0.59901800
H	0.00000000	-3.06510161	-0.59901800
H	2.98825312	0.68204927	-0.59901800
H	2.39639294	-1.91105960	-0.59901800
Pt	-0.00000000	0.00000000	0.13693704

7a

Be	0.00000000	0.00000000	2.17851431
Be	0.00000000	2.08679066	0.57859938
Be	-1.80721372	-1.04339533	0.57859938
Be	0.00000000	-1.64257333	-1.38536053
Be	1.42251023	0.82128667	-1.38536053
Be	1.80721372	-1.04339533	0.57859938
Be	-1.42251023	0.82128667	-1.38536053
H	0.00000000	0.00000000	3.52868131
H	0.00000000	3.39438249	0.91274205
H	2.30261457	1.32941514	-2.27192501
H	-2.93962146	-1.69719124	0.91274205
H	0.00000000	-2.65883028	-2.27192501
H	2.93962146	-1.69719124	0.91274205
H	-2.30261457	1.32941514	-2.27192501
Pt	0.00000000	0.00000000	0.01943531

7b

Be	-1.29425800	-1.86364300	0.02347000
Be	-2.25932100	0.41821500	-0.35119900
Be	-0.96820600	1.96919400	-0.07974700
Be	0.96561000	1.97018700	-0.08042000
Be	2.25909000	0.42089600	-0.35073700
Be	1.29624000	-1.86235400	0.02378900
Be	-0.00122900	0.66032300	1.79373300
H	-2.01139400	-3.01014000	0.05391800
H	-3.49222500	-0.08679000	-0.61109600
H	-2.34727700	2.00532500	-0.31769300

H	-0.00188400	3.07382800	-0.20867100
H	2.34472800	2.00832800	-0.31775200
H	2.01475700	-3.00796600	0.05479500
H	3.49260500	-0.08259900	-0.61061100
Pt	0.00011500	-0.09937500	-0.02510800

7c

Be	-1.41359900	-1.40457700	-0.26832900
Be	-0.17233900	2.30364800	-0.16419400
Be	0.45401500	-2.05980100	-0.16106300
Be	2.24657700	-1.09623600	-0.10397900
Be	-0.75777200	-0.39272300	1.60278700
Be	-3.49770100	-0.68165100	-0.17867300
Be	-1.92586100	0.56252100	-0.17096300
H	3.59910200	-1.04819900	-0.16122900
H	-0.80087700	-2.75013000	-0.36406000
H	1.24766900	1.62570100	0.03725300
H	1.73555900	-2.62462000	-0.24280400
H	-4.76365400	-1.16338100	-0.17555900
H	-3.32544500	0.83818700	-0.17264800
H	-0.41960800	3.62363100	-0.31928700
Pt	0.29479500	0.16120600	-0.01056400

7d

Be	-1.78497500	-1.07644300	-0.59351200
Be	1.44693800	1.41424300	-0.85055100
Be	-1.95639600	-0.26419000	1.20267200
Be	-0.02991600	-1.37069500	-1.55203500
Be	1.74356600	-1.18244400	-0.55012700
Be	-1.23301000	1.71897800	-0.47053000
Be	2.01002900	-0.36266700	1.26321100
H	-1.44511700	-1.84198600	-1.75660800
H	-1.89431000	2.86277700	-0.74874200
H	2.84113500	-1.31213300	0.32657300
H	2.22219700	2.33250400	-1.46833800
H	-2.59376300	0.17895300	2.31294900
H	-2.89394200	-1.17248100	0.24774400
H	2.60036400	-0.03918600	2.43875400
Pt	0.00485300	0.04467200	0.06219400

g. B3LYP/BSI-optimized structures of molecules shown in Fig. S7.

8

Be	0.00000000	2.24786700	0.00000000
Be	1.75745300	1.40152200	0.00000000
Be	2.19150800	-0.50019700	0.00000000
Be	0.97531300	-2.02525800	0.00000000
Be	-0.97531300	-2.02525800	0.00000000
Be	-1.75745300	1.40152200	0.00000000
Be	-2.19150800	-0.50019700	0.00000000
H	-1.34190400	2.78649300	0.00000000
H	1.34190400	2.78649300	0.00000000
H	3.01523100	0.68820700	0.00000000
H	2.41802800	-1.92831300	0.00000000
H	0.00000000	-3.09277400	0.00000000
H	-3.01523100	0.68820700	0.00000000
H	-2.41802800	-1.92831300	0.00000000
Zn	0.00000000	0.00000000	0.00000000

8a

Be	-3.56278900	-0.62325600	0.74636600
Be	-1.12274100	1.77429100	-0.31148700
Be	0.11581700	0.42270600	0.41901800
Be	-2.99633400	-1.03084800	-1.08847400
Be	-1.54775700	-0.63367000	1.05935300
Be	-1.40782900	-0.07681000	-1.05284500
Be	-3.02646600	1.00822400	-0.32269000
H	-2.69459800	-0.98188200	1.87254100
H	-4.08829000	0.70871000	0.67231400
H	-2.38154600	2.20070100	0.19157600
H	-0.06368700	1.84689800	0.66858600
H	-1.74350400	-1.33575400	-1.68057300
H	-3.94842000	-1.65230900	-0.20887000
H	-0.29510600	-0.28419000	1.66026600
Zn	2.31358500	-0.12882400	-0.03242700

8b

Be	-2.18932600	-0.38975600	1.14532000
Be	-3.41335200	0.94342600	0.36075500
Be	-1.61706600	-0.43368700	-1.10899700
Be	-1.50187600	1.45463300	-0.14240800
Be	-0.04022200	0.16514400	-0.00418200

Be	-1.25655200	-1.73237700	0.29590900
Be	-3.36988000	-0.85345700	-0.63085100
H	-2.79331700	-0.58078700	-1.91357500
H	-0.76010900	0.76625400	-1.31990500
H	-3.09380700	0.56984200	1.72467500
H	-2.73362000	2.18983500	-0.03733500
H	-4.39139300	0.15808800	-0.34986900
H	-1.52685300	-1.52678400	1.68076200
H	-0.26830900	1.50705000	0.56346500
Zn	2.30401700	0.01002700	-0.00034700

8c

Be	1.35414100	1.75788500	0.11765200
Be	3.08983100	-1.24703900	0.97748800
Be	3.18586900	-1.00363900	-0.96722800
Be	2.61328000	0.89965900	-1.13103100
Be	-0.20312900	0.56553800	0.19904000
Be	1.41335700	-0.61209200	-0.19779000
Be	2.06796200	0.27765200	1.38551400
H	-0.07923200	1.99937300	0.19701600
H	1.91560700	1.69373800	1.45173400
H	2.26573700	2.27135800	-0.94054000
H	1.83566300	-1.35185300	-1.36825000
H	4.05512400	-1.68489500	0.00424600
H	3.66082200	0.16144100	-1.75498900
H	3.22951100	-0.34926500	2.07447800
Zn	-2.36561600	-0.17639200	-0.03994300

8d

Be	-1.50064300	-0.75808100	-0.49769400
Be	-3.57109000	-0.90992400	-0.92017700
Be	-1.34370100	1.73356400	0.35151400
Be	-1.55758300	0.06878900	1.37843100
Be	0.05968600	0.33608500	-0.22590000
Be	-2.92349700	-1.32422500	0.80788000
Be	-2.93293800	0.96508200	-0.70246200
H	-2.65400500	-0.61369000	1.99830100
H	-0.04432500	1.78759400	-0.24078400
H	-1.52173800	1.48768800	1.76240100
H	-2.45260100	2.28599100	-0.47647500
H	-4.27256400	-1.27679100	0.27420200

H	-0.48465000	-0.34234200	-1.40396200
H	-4.03181400	0.38735400	-1.44206900
Zn	2.35135900	-0.13869900	-0.04126600

9

Be	0.00000000	2.31542400	-0.13669371
Be	1.81027138	1.44364325	-0.13669371
Be	2.25737149	-0.51523031	-0.13669371
Be	1.00462482	-2.08612494	-0.13669371
Be	-1.00462482	-2.08612494	-0.13669371
Be	-1.81027138	1.44364325	-0.13669371
Be	-2.25737149	-0.51523031	-0.13669371
H	-1.35734463	2.81855518	-0.31191971
H	1.35734463	2.81855518	-0.31191971
H	3.04992571	0.69612564	-0.31191971
H	2.44585052	-1.95050070	-0.31191971
H	0.00000000	-3.12836023	-0.31191971
H	-3.04992571	0.69612564	-0.31191971
H	-2.44585052	-1.95050070	-0.31191971
Cd	-0.00000000	0.00000000	0.12522629

9a

Be	0.62065100	0.29727300	-0.18474400
Be	2.17007600	1.59204100	0.51200700
Be	2.19081100	-0.44338700	-0.99796600
Be	3.95748300	-1.00160600	-0.37994800
Be	2.42640700	-0.20778900	1.22367700
Be	2.12943600	-1.83433400	0.40328000
Be	3.85533200	0.88085500	-0.41683900
H	3.35185900	2.19210500	-0.15857600
H	3.49879400	-0.09693100	-1.58832100
H	2.43069500	1.09068100	1.84079200
H	4.97748100	0.02120400	-0.14553200
H	0.80574500	1.73085200	0.13293300
H	2.25862200	-1.50861700	1.78258800
H	1.02404600	0.16189500	-1.56974800
Cd	-1.82808400	-0.01507100	-0.01941700

9b

Be	4.00256900	0.94021900	0.36060600
Be	2.20416700	-0.43047900	-1.10889300

Be	3.95562600	-0.85619200	-0.62993900
Be	1.83695000	-1.72751200	0.29508700
Be	2.77802900	-0.39124900	1.14491600
Be	0.62377300	0.16849900	-0.00595600
Be	2.09140200	1.45375400	-0.14092600
H	2.10651700	-1.52304000	1.68037400
H	1.35277500	0.77242400	-1.32091800
H	3.32430800	2.18816200	-0.03523800
H	4.97974800	0.15410400	-0.35078700
H	3.68422300	0.56644700	1.72485200
H	0.85688700	1.50880300	0.56295700
H	3.38022100	-0.58319400	-1.91311000
Cd	-1.86780700	0.00600300	-0.00016100

9c

Be	4.23729800	-0.47647700	1.04494300
Be	1.85239600	1.75953400	-0.51770600
Be	3.68874700	-1.28698800	-0.68765300
Be	2.32171200	0.17536400	1.03906300
Be	3.71511000	0.88157700	-0.34849600
Be	2.15117200	-0.25617700	-1.11660800
Be	0.42739100	0.55038500	0.03389300
H	2.49647300	-1.70538500	-1.31334000
H	0.95672800	0.34296100	1.38608000
H	3.68484400	0.03420200	-1.55305500
H	3.24398000	-0.36768800	2.07409100
H	0.52421200	1.99680600	-0.09741400
H	4.88654600	0.69110500	0.50724400
H	4.56621100	-1.74036900	0.34208900
Cd	-1.95696500	-0.09667700	0.01801200

9d

Be	2.23402400	-0.03544300	-0.85540700
Be	2.04405300	-0.86260400	1.19192400
Be	3.50339900	1.57792600	-0.05694200
Be	3.42934200	-1.62000200	0.09741000
Be	4.22102500	-0.08265600	-0.91242200
Be	0.49420300	0.00738400	-0.10395000
Be	2.04160600	1.04973100	1.07796300
H	3.25165000	-0.08749700	-1.94290900
H	0.90938100	-0.05710600	-1.44458900

H	2.94543700	-2.03934300	1.35254100
H	2.46553100	0.15108700	2.10373400
H	4.79597100	1.21575500	-0.53022000
H	2.98820600	2.20335900	1.09630800
H	4.73401300	-1.36573800	-0.41561000
Cd	-1.95751700	-0.00328900	-0.04111600

10

Be	0.00000000	2.30731900	0.00000000
Be	-1.80393400	1.43859000	0.00000000
Be	-2.24946900	-0.51342700	0.00000000
Be	-1.00110800	-2.07882200	0.00000000
Be	1.00110800	-2.07882200	0.00000000
Be	1.80393400	1.43859000	0.00000000
Be	2.24946900	-0.51342700	0.00000000
H	1.36231600	2.82887900	0.00000000
H	-1.36231600	2.82887900	0.00000000
H	-3.06109700	0.69867500	0.00000000
H	-2.45480900	-1.95764500	0.00000000
H	0.00000000	-3.13981900	0.00000000
H	3.06109700	0.69867500	0.00000000
H	2.45480900	-1.95764500	0.00000000
Hg	0.00000000	0.00000000	0.00000000

10a

Be	-3.73496000	-1.74973900	-0.03249600
Be	-2.44266800	-0.76423900	1.10911200
Be	-4.22261500	1.24633200	-0.10496700
Be	-2.75704500	-0.08096100	-0.71509500
Be	-2.42485800	1.59820100	0.41787900
Be	-4.88159500	-0.46936200	-0.80406900
Be	-0.92513400	0.30865900	0.61435400
H	-5.53064700	0.79424300	-0.55448500
H	-1.21603200	-0.47997300	1.80309100
H	-3.24629300	-1.93695100	1.28750700
H	-3.66725100	2.32297300	0.67333600
H	-5.17978600	-1.75430800	-0.25187400
H	-2.99072900	1.30635300	-1.05404500
H	-1.08752500	1.75427800	0.88150500
Hg	1.35592200	-0.02952700	-0.05904900

10b

Be	4.61664000	-0.65915700	-0.74421300
Be	2.48291100	-0.05156300	1.05806300
Be	4.05678200	-1.02868600	1.10229200
Be	2.59908200	-0.65390600	-1.04529400
Be	2.22064100	1.79477400	0.29521300
Be	4.11282500	0.99713600	0.30181500
Be	0.96257300	0.45130800	-0.41528300
H	3.73681300	-1.02854200	-1.85841700
H	2.80092200	-1.30592200	1.70210300
H	1.16827700	1.86738200	-0.69158800
H	3.48186100	2.18999000	-0.22663100
H	4.99194100	-1.67791600	0.22538800
H	5.16264200	0.66594400	-0.69501100
H	1.35189800	-0.28608900	-1.64674400
Hg	-1.33625200	-0.04780600	0.01225700

10c

Be	-2.38994200	-1.56239700	1.16243900
Be	-2.96080800	1.75238300	-0.63686400
Be	-3.08773200	0.00557900	-1.57593900
Be	-1.10999600	0.03851800	1.07380800
Be	-3.32061900	0.06808300	0.44756100
Be	-2.19083600	1.75476500	1.10221600
Be	-2.95128300	-1.67217500	-0.72896000
H	-2.74856800	-1.31466400	-2.11836800
H	-0.99897000	1.33075500	1.77485500
H	-2.13344500	2.74536400	0.04050600
H	-1.11556800	-1.22732000	1.75877100
H	-2.50277100	-2.67051800	0.18946900
H	-3.46573800	-0.74497700	1.63698600
H	-2.61764400	1.30282400	-1.96946300
Hg	1.09534500	-0.01200600	-0.05862300

10d

Be	-4.25596600	-1.02496600	-0.74592300
Be	-4.41800200	1.45188500	0.16476300
Be	-2.55742600	-1.26134700	0.35659800
Be	-0.80023100	-0.25436300	0.06436000
Be	-5.72665300	0.05301600	-0.45400100
Be	-2.53271500	0.84100100	-0.27209800

Be	-4.29821000	-0.27351300	1.13616700
H	-3.22738700	-1.09346200	1.62081300
H	-3.24316000	-2.01163100	-0.68147900
H	-5.69439300	1.48651100	-0.51747800
H	-1.12755600	-1.60583300	0.47986200
H	-4.21056700	1.10736700	1.55840300
H	-3.19699400	2.09458500	-0.34641800
H	-5.31332800	-0.66054200	-1.65320200
Hg	1.55462700	0.03195200	-0.01825000