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Supplementary Information

Be_7Au_6: Rare over-delocalization of valence electrons in a star planar hexacoordinate beryllium cluster

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Cartesian coordinates of PBE0/def2-TZVPP-optimized structures shown in Fig. S1–S3.

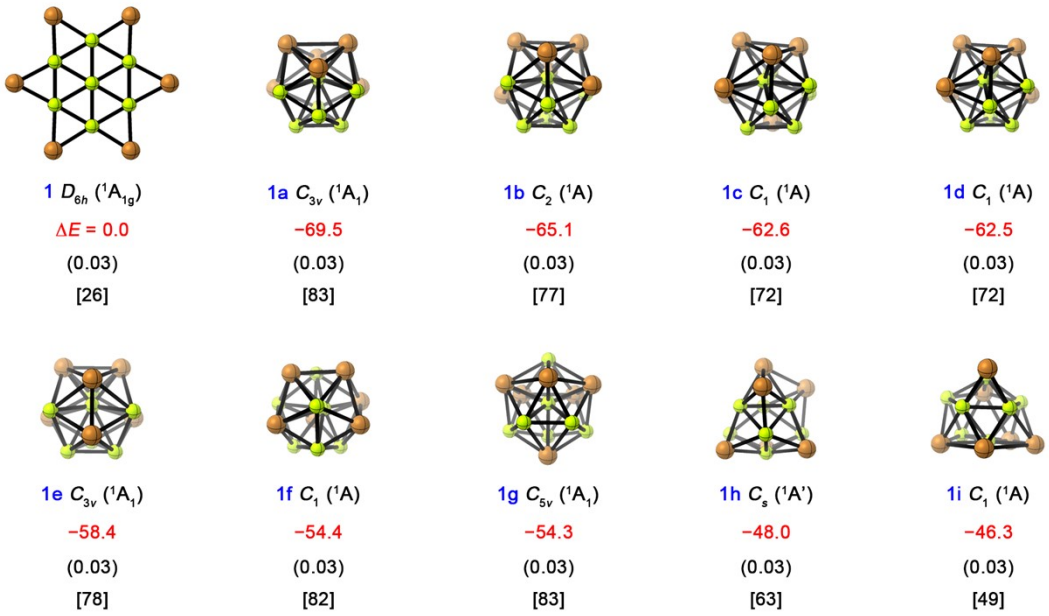


Fig. S1. Structures and relative energies (ΔE, red font, in kcal mol^{-1} at the CCSD(T)+ZPE$_{PBE0}$ level) of Be_7Cu_6 (**1**) and its lowest-lying isomers. T_1 diagnostic values are given within parentheses. The lowest vibrational frequencies in cm^{-1} are given in square brackets.

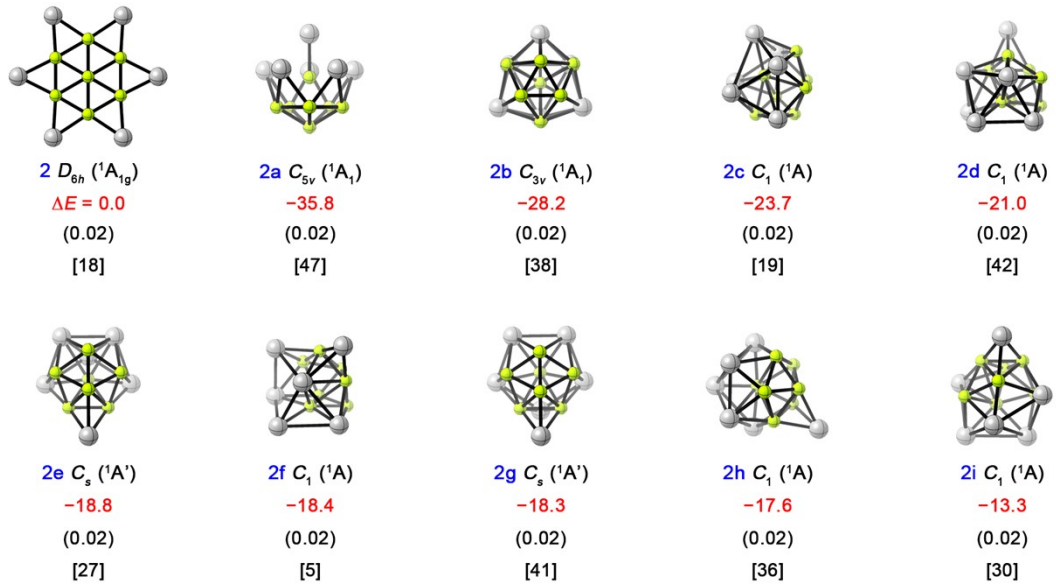


Fig. S2. Structures and relative energies (ΔE, red font, in kcal mol^{-1} at the CCSD(T)+ZPE$_{PBE0}$ level) of Be_7Ag_6 (**2**) and its lowest-lying isomers. T_1 diagnostic values are given within parentheses. The lowest vibrational frequencies in cm^{-1} are given in square brackets.

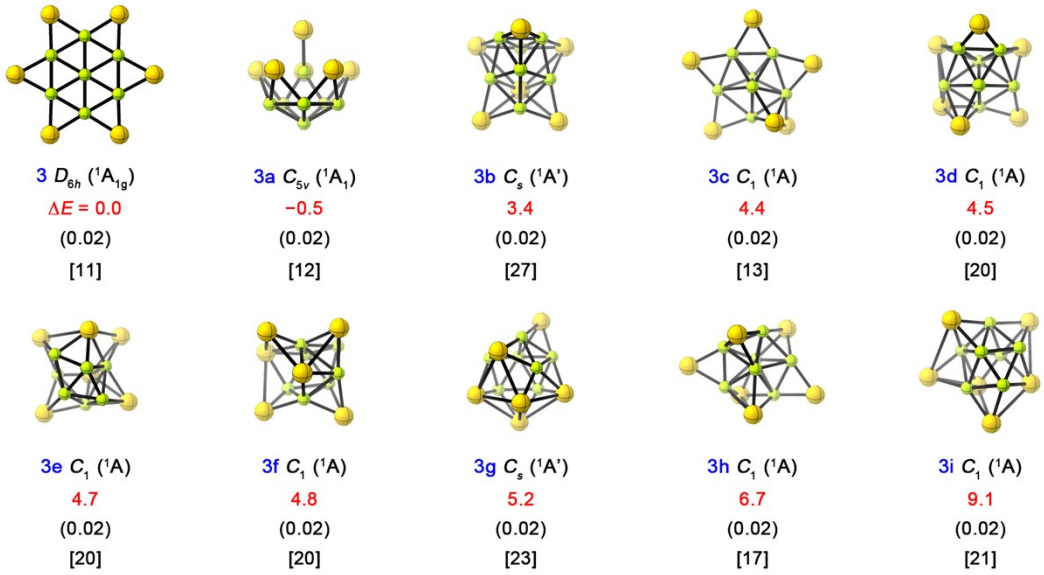


Fig. S3. Structures and relative energies (ΔE, red font, in kcal mol^{-1} at the CCSD(T)+ZPE$_{PBE0}$ level) of Be_7Au_6 (**3**) and its lowest-lying isomers. T_1 diagnostic values are given within parentheses. The lowest vibrational frequencies in cm^{-1} are given in square brackets.

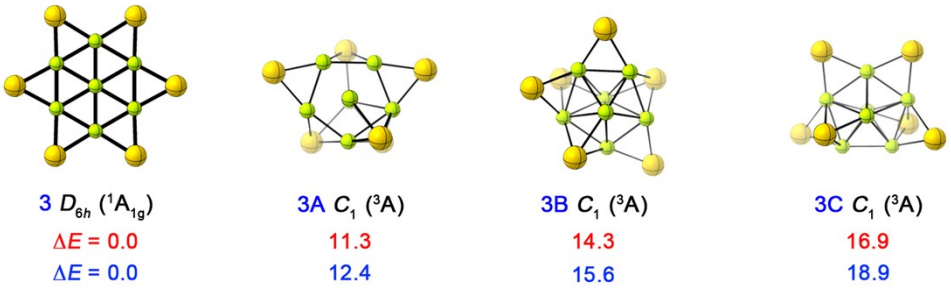


Fig. S4. Structures and relative energies in kcal mol^{-1} of the first three low-lying isomers of Be_7Au_6 (**3**) in the triplet state, calculated at the PBE0/def2-TZVPP (red font) and PBE0/aug-cc-pVTZ(-PP) (blue font) level with zero-point energy correction.

Table S1. The lowest vibrational frequencies (in cm^{-1}) and relative energies in kcal mol^{-1} (ΔE) of the Be_7Au_6 and its lowest-lying isomers. The single-point energies were computed at the CCSD(T)/def2-TZVPP level based on geometries determined different DFT methods considering the dispersion correction. The relative energies are were compared at the CCSD(T)/def2-TZVPP level considering the zero-point energy (ZPE) corrections or Gibbs free energies (GFE) at the corresponding DFT level [abbreviated as CCSD(T)+ZPE_{DFT} or CCSD(T)+GFE_{DFT}].

		3	**3a**	**3b**	**3c**	**3d**
The lowest vibrational frequencies	B2PLYP-D3(BJ)/def2-TZVPP	11	21	27	13	17
	TPSSh-D3(BJ)/def2-TZVPP	13	24	27	12	14
	PBE0-D3(BJ)/def2-TZVPP	11	17	27	13	18
The relative energies	CCSD(T)+ $ZPE_{B2PLYP-D3(BJ)}$	0	**–0.9**	2.7	4.6	4.6
	CCSD(T)+ $ZPE_{TPSSh-D3(BJ)}$	0	**–0.2**	3.1	9.5	4.9
	CCSD(T)+$ZPE_{PBE0-D3(BJ)}$	0	**–0.6**	3.4	4.6	4.6
	CCSD(T)+ $GFE_{B2PLYP-D3(BJ)}$	0	**1.9**	4.5	4.8	5.7
	CCSD(T)+ $GFE_{TPSSh-D3(BJ)}$	0	**2.1**	5.1	10.4	5.7
	CCSD(T)+ $GFE_{PBE0-D3(BJ)}$	0	**1.5**	5.4	4.7	5.6
		3e	**3f**	**3g**	**3h**	**3i**
The lowest vibrational frequencies	B2PLYP-D3(BJ)/def2-TZVPP	18	18	34	17	25
	TPSSh-D3(BJ)/def2-TZVPP	12	12	31	12	21
	PBE0-D3(BJ)/def2-TZVPP	19	19	26	17	21
The relative energies	CCSD(T)+ $ZPE_{B2PLYP-D3(BJ)}$	4.5	4.5	4.8	6.5	8.9
	CCSD(T)+ $ZPE_{TPSSh-D3(BJ)}$	5.2	5.2	5.1	6.9	9.4
	CCSD(T)+$ZPE_{PBE0-D3(BJ)}$	4.8	4.8	5.1	6.7	9.1
	CCSD(T)+ $GFE_{B2PLYP-D3(BJ)}$	6.2	6.2	7.8	8.3	10.5
	CCSD(T)+ $GFE_{TPSSh-D3(BJ)}$	6.6	6.6	7.8	8.2	10.9
	CCSD(T)+ $GFE_{PBE0-D3(BJ)}$	6.5	6.5	7.5	8.4	10.6

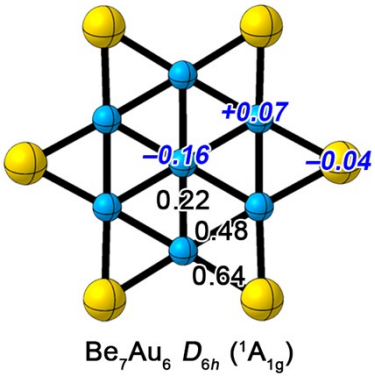


Fig. S5. PBE0/def2-TZVPP-optimized structure of Be_7Au_6 (**3**), and its CM5 charges (blue font, in |e|), Mayer bond orders (black font) are given.

Table S2. Energy components of IQA for the D_{6h} Be_7Au_6 cluster at the PBE0/TZ2P Level. V_{IQA}^{int}, V_{C}^{int}, and V_{XC}^{int} are the interatomic IQA interaction energy and their coulombic and exchange-correlation energy components, respectively, in kcal mol^{-1}.

	Be_7Au_6
V_{IQA}^{int} (Be^c-Be^l)	–26.2
V_{C}^{int} (Be^c-Be^l)	8.2 (19.2%)
V_{XC}^{int} (Be^c-Be^l)	–34.4 (80.8%)
V_{IQA}^{int} (Be^l-Be^l)	–32.6
V_{C}^{int} (Be^l-Be^l)	26.0 (30.7%)
V_{XC}^{int} (Be^l-Be^l)	–58.6 (69.3%)
V_{IQA}^{int} (Be^l-Au)	–104.3
V_{C}^{int} (Be^l-Au)	–53.2 (51.0%)
V_{XC}^{int} (Be^l-Au)	–51.1 (49.0%)

Be^c and Be^l represents the central Be atom and ligand Be atoms, respectively.

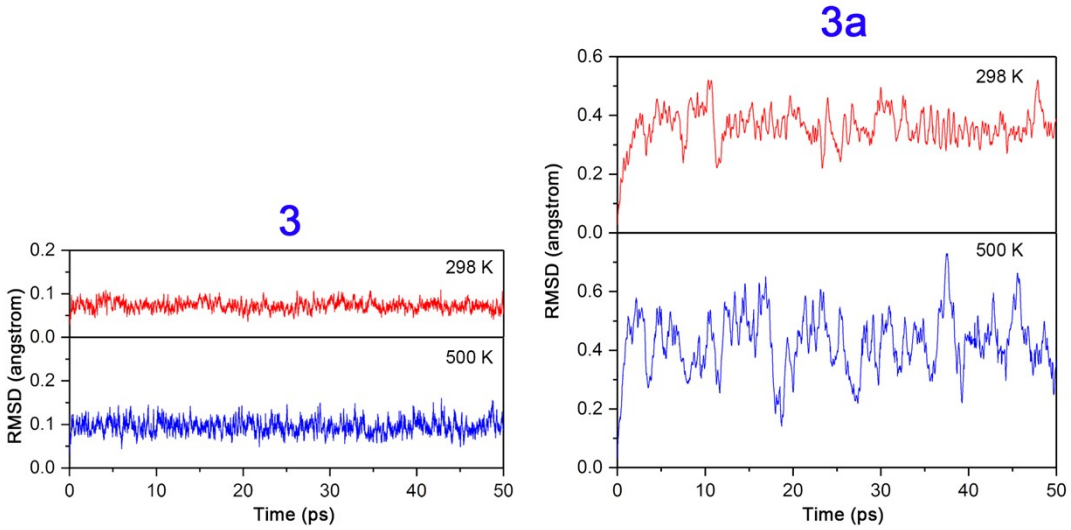


Fig. S6. RMSD (in Å) *versus* simulation time (in ps) for the BOMD simulations of Be_7Au_6 (**3** and **3a**) at the PBE/DZVP level and concerned temperatures.

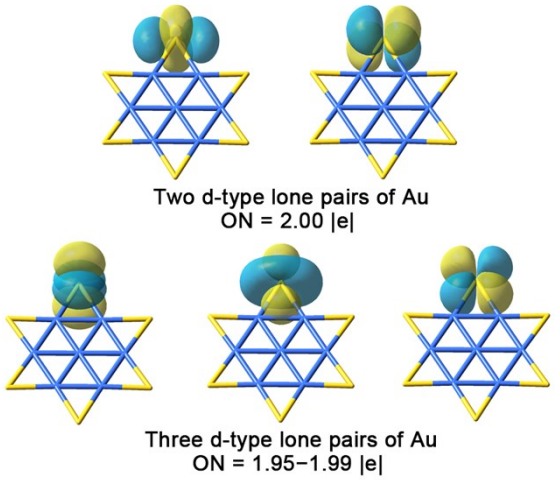
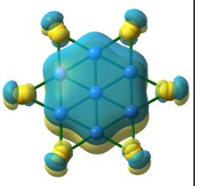
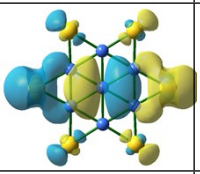
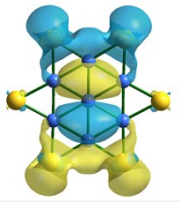
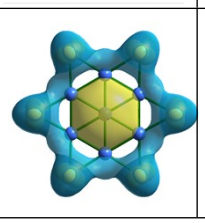
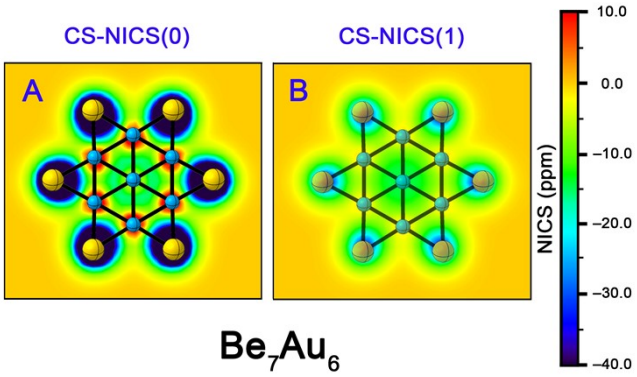


Fig. S7. AdNDP of d-type lone pairs at bridging Au atoms.

Table S3. Orbital composition analysis and ODI for occupied canonical molecular orbitals (CMOs) of Be_7Au_6 and Be_7Cl_6 cluster. Main components are highlighted in bold.

Subsystem	CMO	Be_7Au_6				Be_7Cl_6			
		Be^a	Be^b	Au	ODI	Be^a	Be^b	Cl	ODI
2π aromaticity		**23.9**	**34.2**	**42.0**	9.9	**54.9**	**40.4**	4.7	11.7
6σ aromaticity		13.1	**30.1**	**56.4**	10.3	**16.0**	**61.1**	**22.8**	12.3
		13.1	**30.6**	**56.4**	10.3	**16.0**	**60.2**	**22.9**	12.3
		**28.3**	5.6	**66.0**	9.0	**47.1**	**15.8**	**37.2**	10.4

Be^a represent center Be atom; Be^b represent ligand Be atoms.



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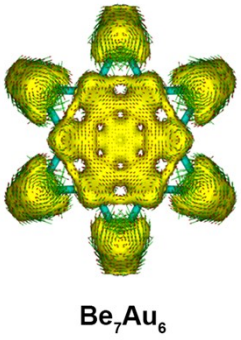

Fig. S9. Top views of the ring current maps of **3** with the iso-surface value of 0.02. The external magnetic field B is applied in the vertical direction, with the induced current vectors represented by red arrows on the iso-surfaces.

Cartesian coordinates of PBE0/def2-TZVPP-optimized structures shown in Fig. S1–S3.

1

Be	0.00000000	2.06552500	0.00000000
Be	1.78879700	1.03276300	0.00000000
Be	0.00000000	0.00000000	0.00000000
Be	0.00000000	-2.06552500	0.00000000
Be	-1.78879700	1.03276300	0.00000000
Be	-1.78879700	-1.03276300	0.00000000
Be	1.78879700	-1.03276300	0.00000000
Cu	3.73428000	0.00000000	0.00000000
Cu	1.86714000	3.23398100	0.00000000
Cu	-1.86714000	3.23398100	0.00000000
Cu	-3.73428000	0.00000000	0.00000000
Cu	-1.86714000	-3.23398100	0.00000000
Cu	1.86714000	-3.23398100	0.00000000

1a

Be	0.00000000	1.19463900	-2.48002300
Be	0.00000000	-2.01150400	-1.27742100
Be	-1.74201300	1.00575200	-1.27742100
Be	-1.03458800	-0.59732000	-2.48002300
Be	0.00000000	0.00000000	-0.39120300
Be	1.74201300	1.00575200	-1.27742100
Be	1.03458800	-0.59732000	-2.48002300
Cu	1.39052700	0.80282100	1.05381500
Cu	0.00000000	2.28162700	-0.51756100
Cu	-1.97594700	-1.14081400	-0.51756100
Cu	1.97594700	-1.14081400	-0.51756100
Cu	-1.39052700	0.80282100	1.05381500
Cu	0.00000000	-1.60564300	1.05381500

1b

Be	0.06421600	1.69921000	1.88588900
Be	-1.75047800	1.12631700	0.81621200
Be	1.03557200	-0.03342000	2.52905400
Be	-1.03557200	0.03342000	2.52905400
Be	-0.06421600	-1.69921000	1.88588900
Be	1.75047800	-1.12631700	0.81621200
Be	0.00000000	0.00000000	0.35700300
Cu	-2.00615700	-1.13365200	0.89225500
Cu	-1.40962200	0.08064900	-1.26927800
Cu	0.00000000	2.08050600	-0.36913700
Cu	1.40962200	-0.08064900	-1.26927800

Cu	2.00615700	1.13365200	0.89225500
Cu	0.00000000	-2.08050600	-0.36913700

1c

Be	-0.39557000	0.43514800	-2.32186800
Be	1.08853300	-1.05951300	-2.23853600
Be	-0.06333800	-0.10388900	-0.28840500
Be	0.73165700	-2.35258500	-0.63361300
Be	1.55892700	0.84630600	-1.47506400
Be	0.95686400	-1.23186000	1.24046600
Be	-0.88884000	-1.56100300	-1.74857000
Cu	1.57924300	0.98784600	0.83478600
Cu	-2.13950600	0.12431000	-0.82138900
Cu	-0.83426900	0.41387300	1.61448900
Cu	2.43933300	-0.95345600	-0.46269900
Cu	-1.15825600	-1.88665400	0.50101000
Cu	-0.29871500	2.00751500	-0.63646000

1d

Be	0.39619500	0.43333500	-2.32155200
Be	-1.08739100	-1.06054300	-2.23826300
Be	0.89003200	-1.56201900	-1.74753600
Be	0.06406000	-0.10357600	-0.28819000
Be	-0.73115700	-2.35328700	-0.63294900
Be	-1.55846000	0.84480700	-1.47541800
Be	-0.95727800	-1.23172600	1.24091000
Cu	-1.57935000	0.98836700	0.83417600
Cu	2.14077000	0.12396100	-0.82121000
Cu	0.29809300	2.00739100	-0.63766600
Cu	0.83245400	0.41444900	1.61544800
Cu	1.15867700	-1.88536900	0.50201000
Cu	-2.43905800	-0.95459100	-0.46337900

1e

Be	0.00000000	2.12377600	0.18974200
Be	-1.06210400	-0.61309200	2.18323400
Be	1.83924400	-1.06188800	0.18974200
Be	0.00000000	0.00000000	0.20493000
Be	0.00009900	1.22635500	2.18323400
Be	-1.83924400	-1.06188800	0.18974200
Be	1.06200500	-0.61326300	2.18323400
Cu	1.29600800	0.74524100	-1.36129200
Cu	-0.00260600	-1.49499700	-1.36129200
Cu	-1.90472500	1.09996500	1.02456300

Cu	-1.29340200	0.74975600	-1.36129200
Cu	-0.00023500	-2.19952200	1.02456300
Cu	1.90496000	1.09955800	1.02456300

1f

Be	0.63824200	0.11336600	2.23914100
Be	-0.21890800	0.52768600	-1.88824800
Be	1.10639400	-1.55045300	0.87033600
Be	1.51131800	1.53000600	-0.77923000
Be	-1.11133300	1.25086300	1.56348700
Be	-0.04679500	0.09350900	0.14196200
Be	0.90419000	1.95908900	1.22102700
Cu	-0.57786000	2.29022900	-0.42136000
Cu	1.66404500	-0.67942200	-1.24477300
Cu	-0.59374400	-1.70004800	-0.90472600
Cu	2.39593100	0.31897000	0.90350100
Cu	-1.14213800	-1.10351300	1.57061000
Cu	-2.13011100	0.33253300	-0.36787000

1g

Be	-1.09359100	1.50520000	1.30953400
Be	-1.76946800	-0.57493500	1.30953400
Be	1.76946800	-0.57493500	1.30953400
Be	0.00000000	0.00000000	0.10668000
Be	1.09359100	1.50520000	1.30953400
Be	0.00000000	0.00000000	-1.93760300
Be	0.00000000	-1.86052900	1.30953400
Cu	0.00000000	2.11195000	-0.64206700
Cu	0.00000000	0.00000000	2.55975000
Cu	1.24137300	-1.70860400	-0.64206700
Cu	2.00858400	0.65262900	-0.64206700
Cu	-2.00858400	0.65262900	-0.64206700
Cu	-1.24137300	-1.70860400	-0.64206700

1h

Be	1.72203100	0.00097500	0.28862700
Be	0.57386100	1.71290500	0.95638100
Be	-0.14242100	1.08300000	-1.13976700
Be	0.57699400	-1.71083800	0.95496500
Be	-0.80118300	-0.00040100	0.79344300
Be	1.48707200	0.00087700	-1.91836000
Be	-0.14121000	-1.08388200	-1.13964400
Cu	0.85989100	0.00123100	2.33881500
Cu	1.93148800	1.89803100	-0.83136500

Cu	-1.53076100	-2.04585400	0.30163400
Cu	1.93404100	-1.89627300	-0.83324300
Cu	-1.53327600	2.04366600	0.29864900
Cu	-2.11312700	-0.00116500	-1.10837300

1i

Be	0.33837700	-1.83679300	0.76600500
Be	-0.05293300	-1.91111700	-1.32110900
Be	-0.28002500	0.76754200	-0.45747000
Be	1.55033400	-0.71434400	-0.62857500
Be	1.01663300	0.16785000	1.23307000
Be	-1.00904100	-0.42925000	1.56452500
Be	-1.56044900	-0.46524600	-1.64250500
Cu	-1.78950200	-1.91027800	0.08704900
Cu	-2.41345200	0.58867300	0.20786400
Cu	2.48434200	-1.49634700	1.23884700
Cu	0.48282500	0.06631000	-2.40076200
Cu	1.70707800	1.53483300	-0.48554300
Cu	-0.47169000	1.82665100	1.41958800

2

Be	0.00000000	2.07654800	0.00000000
Be	1.79834400	-1.03827400	0.00000000
Be	-1.79834400	-1.03827400	0.00000000
Be	1.79834400	1.03827400	0.00000000
Be	0.00000000	0.00000000	0.00000000
Be	-1.79834400	1.03827400	0.00000000
Be	0.00000000	-2.07654800	0.00000000
Ag	-1.93792400	3.35658200	0.00000000
Ag	-1.93792400	-3.35658200	0.00000000
Ag	-3.87584700	0.00000000	0.00000000
Ag	1.93792400	-3.35658200	0.00000000
Ag	1.93792400	3.35658200	0.00000000
Ag	3.87584700	0.00000000	0.00000000

2a

Be	1.05244300	1.44856300	-2.05750200
Be	0.00000000	0.00000000	-3.08925600
Be	0.00000000	-1.79052200	-2.05750200
Be	-1.05244300	1.44856300	-2.05750200
Be	0.00000000	0.00000000	-0.49275900
Be	-1.70288800	-0.55330200	-2.05750200
Be	1.70288800	-0.55330200	-2.05750200
Ag	0.00000000	2.45121100	-0.12010400

Ag	-2.33124000	0.75746600	-0.12010400
Ag	-1.44078500	-1.98307100	-0.12010400
Ag	1.44078500	-1.98307100	-0.12010400
Ag	2.33124000	0.75746600	-0.12010400
Ag	0.00000000	0.00000000	1.78090300

2b

Be	0.00000000	1.18222900	-2.61631200
Be	-1.73929700	1.00418400	-1.41514100
Be	-1.02384100	-0.59111500	-2.61631200
Be	0.00000000	-2.00836800	-1.41514100
Be	0.00000000	0.00000000	-0.32565000
Be	1.73929700	1.00418400	-1.41514100
Be	1.02384100	-0.59111500	-2.61631200
Ag	0.00000000	2.56422100	-0.70089100
Ag	-2.22068100	-1.28211100	-0.70089100
Ag	1.63892800	0.94623500	1.05323200
Ag	-1.63892800	0.94623500	1.05323200
Ag	2.22068100	-1.28211100	-0.70089100
Ag	0.00000000	-1.89247100	1.05323200

2c

Be	-0.83391600	-0.97722200	2.54987600
Be	0.63632300	1.87383700	1.18134800
Be	0.16341100	-0.03367500	0.20518300
Be	-1.14076900	1.02862200	2.06135000
Be	-0.73032000	-2.00720300	0.68811100
Be	1.03505500	-1.50201700	1.84839300
Be	0.70523700	0.37359600	2.71044400
Ag	-1.42484600	1.80927400	-0.16302000
Ag	-2.62777200	-0.54243200	1.06029500
Ag	2.51876200	0.26358400	1.20029000
Ag	1.33031600	1.46249600	-1.13770600
Ag	-1.23313700	-0.98588800	-1.43694300
Ag	1.45071700	-1.90115600	-0.47991200

2d

Be	0.15945900	-0.91597200	2.68629600
Be	-1.42618900	-1.12650400	-0.27389700
Be	-1.70821300	-0.90708100	1.83894700
Be	0.37421000	0.19066500	0.75770200
Be	-0.21632700	-2.21308700	1.06750300
Be	-1.84245400	0.85199100	0.61855900
Be	-0.81500300	0.87399400	2.44480600

Ag	2.08785500	0.87210600	-0.63925700
Ag	2.05613800	-1.40077200	1.31834700
Ag	-0.70010400	0.80786200	-1.49278900
Ag	-3.61234700	-0.74552400	0.33095000
Ag	-0.01690700	2.48516300	0.85857100
Ag	0.65128100	-1.74258000	-1.15368700

2e

Be	-0.83285600	-1.70312200	1.36717100
Be	-0.12393700	-0.00011100	2.45131400
Be	-2.00515400	0.00074600	1.59812200
Be	-0.83120100	1.70321400	1.36722200
Be	-1.97755300	-1.04488800	-0.28143800
Be	-0.13788100	0.00030800	-0.40799000
Be	-1.97678100	1.04739100	-0.28130800
Ag	1.91880700	-0.00012200	-1.35634400
Ag	-0.09743400	2.30274500	-0.95074100
Ag	-4.01953200	0.00100700	0.23489700
Ag	1.48403700	-1.40468500	1.26285200
Ag	-0.09968500	-2.30267700	-0.95012300
Ag	1.48490200	1.40343100	1.26472700

2f

Be	1.22009200	-1.46969200	0.93072300
Be	-0.71112100	0.81389000	0.85146500
Be	-1.18389100	0.01184200	2.74944800
Be	0.79475300	-0.56209200	2.79016900
Be	-0.61953900	-1.78970400	1.86381100
Be	1.70363200	0.58633100	1.28535000
Be	0.32360300	1.41567800	2.58915300
Ag	0.68985400	2.63681700	0.51077300
Ag	3.21881600	-0.70704000	0.02941700
Ag	-2.48503700	-0.72616100	0.81370000
Ag	-0.43140400	-2.54208700	-0.36256000
Ag	-1.80112600	1.36602800	-1.10080200
Ag	0.67889400	0.05701700	-1.00202900

2g

Be	-1.07869300	0.00217600	-2.25566600
Be	-0.49106300	-0.00058400	0.35024700
Be	1.54433200	1.07111700	-0.28337400
Be	-0.07378100	-1.73148300	-1.49098500
Be	0.96635800	0.00022000	-2.06430300
Be	1.54357400	-1.07597400	-0.28622700

Be	-0.07071400	1.73250700	-1.48752700
Ag	-0.09439500	2.33583400	0.89248500
Ag	-2.26324900	-1.41844200	-0.69062700
Ag	3.22955400	0.00161800	-1.65798100
Ag	-2.26065400	1.42333900	-0.68809100
Ag	-0.09725800	-2.33866700	0.88763000
Ag	1.28685100	-0.00351000	1.89640000

2h

Be	-0.49732100	-0.52495900	2.17239700
Be	0.12284900	-0.43125300	-0.48543600
Be	0.33493200	-2.24987100	1.23119800
Be	-1.81559900	-0.96736200	-1.09402500
Be	-1.77191000	0.31412600	0.70147900
Be	-0.52962400	-2.51973800	-0.68366600
Be	-1.62655700	-1.78548100	0.93052300
Ag	-3.75258400	-0.92739000	0.24522800
Ag	1.75247600	-2.01921600	-0.88916100
Ag	-0.01615300	1.71055700	1.30167300
Ag	1.80978000	1.03345500	-1.01996000
Ag	1.80859900	-0.41270700	1.57004000
Ag	-1.10992900	1.31015600	-1.44377400

2i

Be	1.36122800	0.11265900	0.75473300
Be	-0.78710700	0.45093200	-0.84956100
Be	-0.34340400	1.23174900	1.23862400
Be	1.93584500	0.39021300	-1.34930000
Be	0.41937300	1.50873700	-2.16739200
Be	1.06830200	1.96963600	-0.22267500
Be	0.32639300	-0.61264100	-2.28886500
Ag	-0.30180100	-1.18352800	1.65854100
Ag	-1.29998500	-1.86050700	-1.09151300
Ag	-1.08950000	2.77937800	-0.66362600
Ag	3.34470700	1.20174700	0.39913900
Ag	-2.51838000	0.47173200	0.71053000
Ag	1.52618400	-1.83871800	-0.59737400

3

Be	0.00000000	2.10103000	0.00000000
Be	1.81954500	1.05051500	0.00000000
Be	-1.81954500	1.05051500	0.00000000
Be	-1.81954500	-1.05051500	0.00000000
Be	0.00000000	0.00000000	0.00000000

Be	1.81954500	-1.05051500	0.00000000
Be	0.00000000	-2.10103000	0.00000000
Au	3.76802100	0.00000000	0.00000000
Au	1.88401100	3.26320200	0.00000000
Au	-3.76802100	0.00000000	0.00000000
Au	-1.88401100	-3.26320200	0.00000000
Au	1.88401100	-3.26320200	0.00000000
Au	-1.88401100	3.26320200	0.00000000

3a

Be	2.35955500	0.64431300	1.06826700
Be	0.19064400	0.26096600	0.00000000
Be	0.75477000	1.89155100	1.72842000
Be	1.79986800	2.32207700	0.00000000
Be	2.35955500	0.64431300	-1.06826700
Be	0.75477000	1.89155100	-1.72842000
Be	-0.23867500	2.66061800	0.00000000
Au	2.11808400	-1.35253700	0.00000000
Au	-1.46282700	1.43729700	1.47818300
Au	0.75477000	-0.28681300	-2.38853300
Au	-1.46282700	1.43729700	-1.47818300
Au	-1.10604500	-1.47073000	0.00000000
Au	0.75477000	-0.28681300	2.38853300

3b

Be	0.16603300	2.10319300	1.07014400
Be	1.52407500	0.90700500	0.00000000
Be	0.46590600	-0.01614700	1.52151400
Be	0.46590600	-0.01614700	-1.52151400
Be	-1.26128200	1.02077800	0.00000000
Be	1.46438700	-1.24296400	0.00000000
Be	0.16603300	2.10319300	-1.07014400
Au	-1.06174200	-1.25426100	0.00000000
Au	-1.43006300	1.05760000	-2.29397200
Au	0.96610100	-2.16757500	1.99255700
Au	1.83821800	3.22819000	0.00000000
Au	0.96610100	-2.16757500	-1.99255700
Au	-1.43006300	1.05760000	2.29397200

3c

Be	-0.23011500	0.00107900	0.76860700
Be	-0.93956400	1.78351400	-0.32156300
Be	-2.13848900	-0.00681200	-0.30115800
Be	1.32269900	1.12065800	-0.22469300

Be	1.32985900	-1.11044000	-0.22269500
Be	-0.92597500	-1.78996900	-0.32002500
Be	-0.28435800	-0.00088500	-1.14752200
Au	0.75459000	-3.27405000	-0.13215700
Au	-3.12427300	2.01005600	-0.09548300
Au	1.83692100	0.00641800	1.78687600
Au	0.73045100	3.27969500	-0.13341500
Au	3.00584100	0.00925000	-1.23933300
Au	-3.10905200	-2.03122500	-0.09691600

3d

Be	-0.29462800	-0.01924000	1.34421800
Be	0.35345000	-1.66453800	0.23951900
Be	1.59737300	0.21339700	0.19540100
Be	0.14259900	1.86085000	0.56942800
Be	-1.87746000	-1.05927800	0.33704100
Be	-1.95456100	1.02971000	0.57715100
Be	-0.58192900	0.12792300	-0.72620000
Au	-1.07198400	-2.00195100	-1.54557000
Au	2.25161300	-1.63465000	-0.93893600
Au	-3.72807400	-0.17393600	1.22898200
Au	2.26340900	2.33393100	0.09549100
Au	1.63011000	-0.92591000	2.15898100
Au	-1.21266200	2.37776700	-1.12738100

3e

Be	0.30362800	-1.65248700	-2.18504200
Be	1.31399200	-1.58982400	-0.29941800
Be	1.66884100	-0.15814600	-1.88525100
Be	-0.19387800	0.26722900	-2.65635200
Be	-0.90750400	-0.59852500	-0.69775400
Be	1.46365500	0.58903800	0.19286600
Be	0.73494700	1.76515400	-1.50603300
Au	-2.51322000	-0.06301700	0.74568100
Au	3.35301600	-0.51050100	-0.31050000
Au	0.86591400	2.70408700	0.50426500
Au	-0.58965400	-2.92211900	-0.58274900
Au	-1.50541500	1.58120300	-1.38355800
Au	0.16740200	-0.71990300	1.48443100

3f

Be	-0.91851500	0.58073600	-0.69869200
Be	-0.18972000	-0.27370400	-2.65455700
Be	0.76859500	-1.75400100	-1.50641000

Be	0.27184000	1.65573900	-2.18667500
Be	1.46875400	-0.56057600	0.19243600
Be	1.66450900	0.18813700	-1.88599500
Be	1.28513900	1.61583200	-0.30208300
Au	3.34105800	0.56823200	-0.30981900
Au	0.91971900	-2.68874700	0.50403100
Au	-1.47537300	-1.61138800	-1.37975700
Au	0.15380200	0.72987300	1.48354000
Au	-0.64574900	2.91049200	-0.58645300
Au	-2.51374100	0.01801000	0.74627900

3g

Be	-0.24244400	0.00091800	-2.29283200
Be	1.76242000	0.00134700	-1.57291600
Be	2.04907100	1.05490600	0.27793000
Be	0.54331200	-0.00077600	1.35335200
Be	0.59263100	-1.68994700	-1.16171600
Be	2.04979400	-1.05435200	0.27644900
Be	0.59081100	1.69068900	-1.15897200
Au	-1.64572000	-0.00100700	1.32586800
Au	0.30147900	2.27281300	1.03196600
Au	-1.60222200	-1.49300700	-1.27099200
Au	3.87499200	0.00161400	-0.62730100
Au	-1.60374300	1.49367800	-1.27209300
Au	0.30328600	-2.27423200	1.02919600

3h

Be	0.00000000	1.80917000	1.00129000
Be	0.00000000	0.00000000	2.24327500
Be	-1.05972600	0.02612500	0.42535600
Be	0.19948200	-1.32146200	-1.05917500
Be	0.00000000	-1.80917000	1.00129000
Be	1.05972600	-0.02612500	0.42535600
Be	-0.19948200	1.32146200	-1.05917500
Au	1.67225900	0.32554900	-1.83422900
Au	-1.81619200	1.37667200	2.22660100
Au	-1.67225900	-0.32554900	-1.83422900
Au	-0.36832400	-3.41767000	-0.46777000
Au	0.36832400	3.41767000	-0.46777000
Au	1.81619200	-1.37667200	2.22660100

3i

Be	-0.49870100	-0.96892000	-1.95670300
Be	1.20120300	-0.77757600	-0.54632900

Be	0.92601500	1.15154100	0.61583000
Be	-0.72694100	2.22578700	-0.21723400
Be	-1.81309000	0.68520300	-1.34133900
Be	-1.05523500	0.46347800	0.80675600
Be	0.19029600	0.92459500	-1.57788500
Au	-2.11493700	-1.31423700	-0.34665200
Au	0.44071700	-2.80798000	-1.10110400
Au	-2.86471600	1.80827000	0.46168400
Au	2.94339800	0.18465100	0.52417100
Au	0.42125000	-0.91266700	1.70808000
Au	1.26423600	2.85441300	-1.03266400