

**Probing the structure and electronic properties of anionic and
neutral BiAu_n^u ($n=2-20$, $u=0, -1$) clusters: A pyramid-like BiAu_{13}
cluster**

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Electronic supplementary information (ESI) available: The metastable isomers of neutral and anionic BiAu_n clusters, the electronic states, symmetries of the lowest-energy structures of neutral and anionic BiAu_n clusters, the cartesian coordinates and vibrational frequency of lowest-energy geometry BiAu_{13} with C_{4v} and the metastable structures of BiAu_{13} (C_1 and C_2).

Table S1 Total energies of the BiAu₁₃ (*C*_{4v}), BiAu₁₃ (*C*₁) and BiAu₁₃ (*C*₂) derived by the HF, B3PW91 and MP2 methods are compiled on lanl2tz(f) level.

Cluster	Symmetry	Energy/a.u.		
		HF	B3PW91	MP2
BiAu ₁₃	<i>C</i> _{4v}	-1754.6087982	-1767.7088871	-1754.578627
	<i>C</i> ₁	-1754.607688	-1767.7088076	-1754.569048
	<i>C</i> ₂	-1754.608015	-1767.7088836	-1754.569049

Table S2 Cartesian coordinates of optimized lowest-energy geometries of BiAu₁₃ with C_{4v} symmetry, the metastable structure of BiAu₁₃ (C_1) and the metastable structure of BiAu₁₃ (C_2) at the B3PW91/lanl2tz(f) level.

C_{4v}				C_1				C_2			
Au	0.00000000	2.06847700	1.53402300	Au	1.38841900	1.53093500	1.53380600	Au	1.38826695	1.53107273	1.53380631
Au	0.00000000	3.76730400	-0.66477700	Au	2.53197200	2.79010900	-0.66306100	Au	2.53169504	2.79036036	-0.66306057
Au	1.40104000	1.40104000	1.00580500	Au	0.09705500	-1.97837300	-1.00407300	Au	0.09725134	-1.97836326	-1.00407295
Au	-3.76730400	0.00000000	-0.66477700	Au	-2.78887600	2.53201100	-0.66701700	Au	-2.78912732	2.53173427	-0.66701676
Au	3.76730400	0.00000000	0.66477700	Au	2.79076600	-2.53131500	-0.66294300	Au	2.78912732	-2.53173427	-0.66701676
Au	0.00000000	0.00000000	3.04746200	Au	0.00043900	-0.00019100	-3.04565100	Au	0.00000000	-0.00000000	-3.04565083
Au	-2.06847700	0.00000000	1.53402300	Au	-1.53306900	1.38986900	1.53281800	Au	-1.53320704	1.38971677	1.53281821
Au	0.00000000	-2.06847700	1.53402300	Au	-1.39098100	-1.53186800	1.53270700	Au	-1.38826695	-1.53107273	1.53380631
Au	0.00000000	-3.76730400	-0.66477700	Au	-2.53002600	-2.79060700	-0.66708900	Au	-2.53169504	-2.79036036	-0.66306057
Au	-1.40104000	-1.40104000	-1.00580500	Au	-1.98190600	-0.09612000	-1.00568400	Au	-1.98189647	-0.09631661	-1.00568390
Au	1.40104000	1.40104000	-1.00580500	Au	1.98339100	0.09622500	-1.00583600	Au	1.98189647	0.09631661	-1.00568390
Au	2.06847700	0.00000000	1.53402300	Au	1.53060700	-1.38899800	1.53402900	Au	1.53320704	-1.38971677	1.53281821
Au	-1.40104000	1.40104000	-1.00580500	Au	-0.09500400	1.97845700	-1.00438500	Au	-0.09725134	1.97836326	-1.00407295
Bi	0.00000000	0.00000000	3.42050600	Bi	-0.00265200	-0.00012800	3.41925000	Bi	0.00000000	0.00000000	3.41925017

Table S3 The vibrational frequency of optimized lowest-energy geometry BiAu₁₃ with C_{4v} , the metastable structure of BiAu₁₃ (C_1) and BiAu₁₃ (C_2) cluster at the B3PW91/lanl2tz(f) level.

Clusters	Vibrational frequency
BiAu ₁₃ (C_{4v})	28.20, 34.62, 37.98, 44.06, 45.05, 47.08, 49.83, 58.26, 58.34, 67.81, 68.26, 73.02, 80.53, 81.74, 82.32, 97.54, 98.65, 99.30, 107.42, 111.27, 126.57, 131.75, 152.31, 159.94, 168.58
BiAu ₁₃ (C_1)	28.07, 34.82, 37.47, 43.59, 44.57, 45.02, 46.67, 49.60, 58.41, 62.30, 67.98, 72.96, 73.14, 80.14, 81.60, 82.43, 97.45, 98.54, 99.28, 106.73, 111.17, 126.13, 131.31, 152.03, 159.96, 168.26
BiAu ₁₃ (C_2)	28.22, 34.68, 37.93, 43.59, 44.10, 45.20, 47.05, 49.80, 58.25, 67.84, 72.97, 73.11, 80.41, 81.78, 82.55, 97.78, 98.77, 99.34, 107.45, 111.35, 126.52, 131.53, 152.25, 160.16, 168.61

Table S4 The natural populations charge (NPC) of Bi atoms and natural electron configuration (NEC) of Bi atom of the lowest-energy $\text{BiAu}_n^u (n=2-20; u=0, -1)$ clusters.

n	BiAu_n		n	BiAu_n^{-1}	
	NPC	NEC		NPC	NEC
2	0.13	$6S^{1.91}6p^{2.95}$	2	-0.39	$6S^{1.88}6p^{3.50}$
3	0.06	$6S^{1.86}6p^{3.06}$	3	-0.05	$6S^{1.93}6p^{3.12}$
4	0.12	$6S^{1.84}6p^{3.03}$	4	-0.07	$6S^{1.83}6p^{3.23}$
5	0.13	$6S^{1.82}6p^{3.04}$	5	-0.08	$6S^{1.81}6p^{3.26}$
6	0.15	$6S^{1.80}6p^{3.05}$	6	-0.09	$6S^{1.79}6p^{3.30}$
7	0.14	$6S^{1.72}6p^{3.03}$	7	0.20	$6S^{1.82}6p^{2.96}$
8	0.24	$6S^{1.79}6p^{2.97}$	8	0.04	$6S^{1.77}6p^{3.19}$
9	0.11	$6S^{1.77}6p^{3.12}$	9	0.02	$6S^{1.76}6p^{3.22}$
10	0.36	$6S^{1.76}6p^{2.87}$	10	0.05	$6S^{1.73}6p^{3.21}$
11	0.16	$6S^{1.74}6p^{3.08}$	11	0.10	$6S^{1.73}6p^{3.16}$
12	0.17	$6S^{1.73}6p^{3.09}$	12	0.07	$6S^{1.71}6p^{3.21}$
13	0.15	$6S^{1.73}6p^{3.12}$	13	0.15	$6S^{1.72}6p^{3.12}$
14	0.34	$6S^{1.71}6p^{2.94}$	14	0.20	$6S^{1.70}6p^{3.09}$
15	0.41	$6S^{1.71}6p^{2.87}$	15	0.23	$6S^{1.70}6p^{3.07}$
16	0.38	$6S^{1.70}6p^{2.91}$	16	0.36	$6S^{1.72}6p^{2.91}$
17	0.40	$6S^{1.71}6p^{2.88}$	17	0.23	$6S^{1.69}6p^{3.07}$
18	0.26	$6S^{1.71}6p^{3.02}$	18	0.22	$6S^{1.70}6p^{3.07}$
19	0.24	$6S^{1.72}6p^{3.03}$	19	0.06	$6S^{1.71}6p^{3.22}$
20	0.37	$6S^{1.74}6p^{2.86}$	20	0.15	$6S^{1.69}6p^{3.16}$

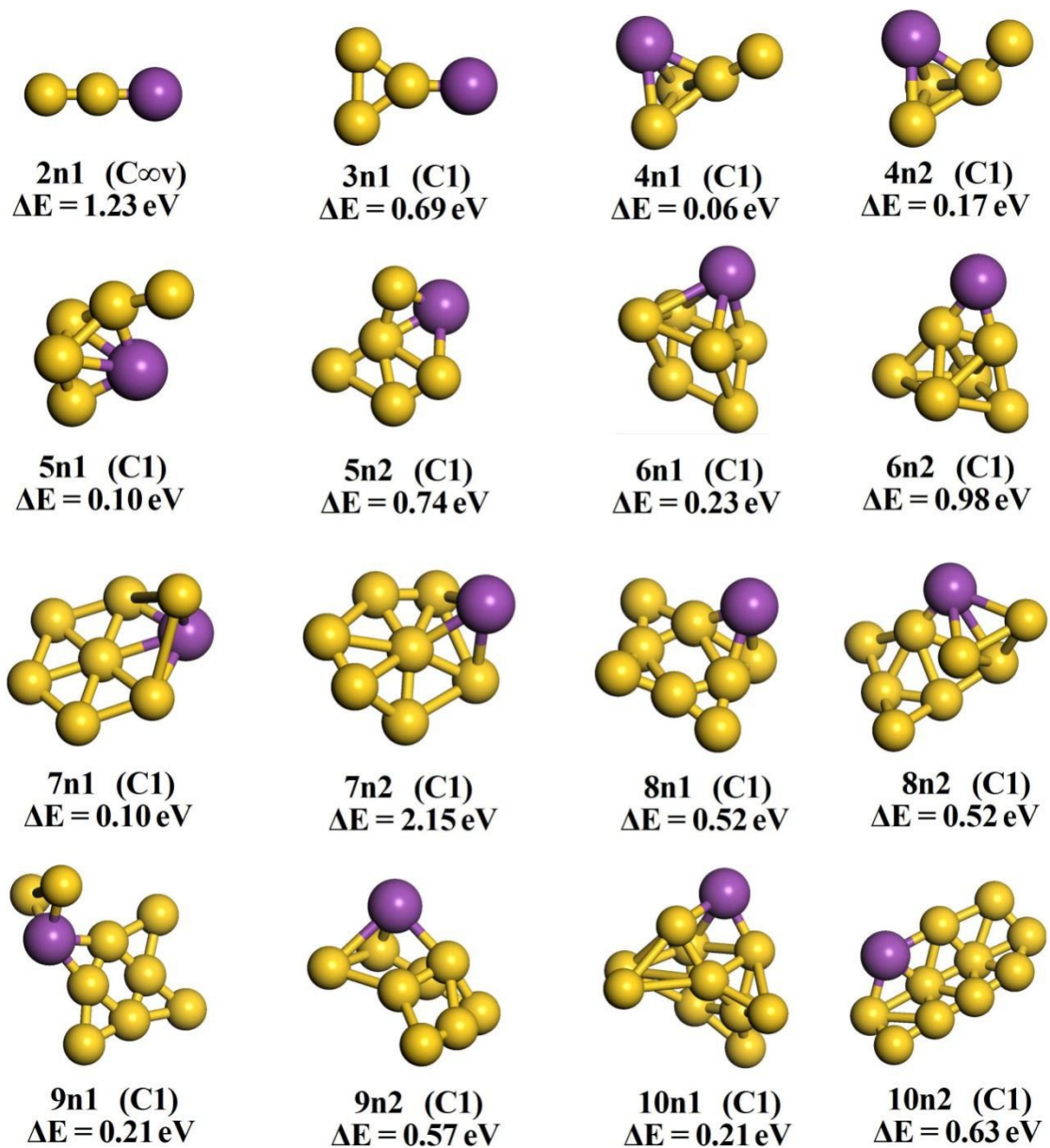


Fig. S1 The metastable structures of the BiAu_n ($n=2-10$) clusters, together with the symmetry and relative energy corresponding to the neutral ground state structures.

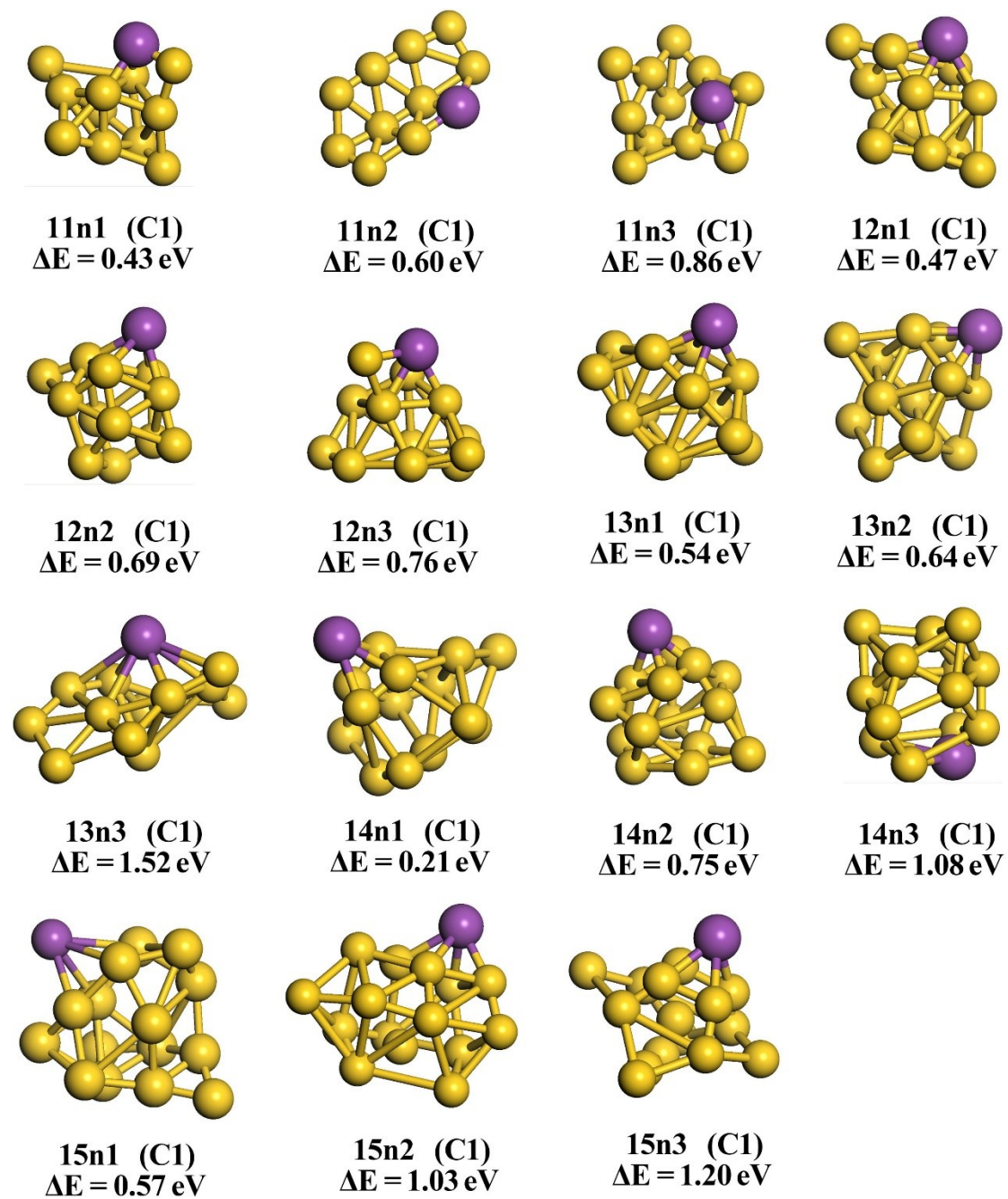


Fig. S2 The metastable structures of the BiAu_n ($n=11-15$) clusters, together with the symmetry and relative energy corresponding to the neutral ground state structures

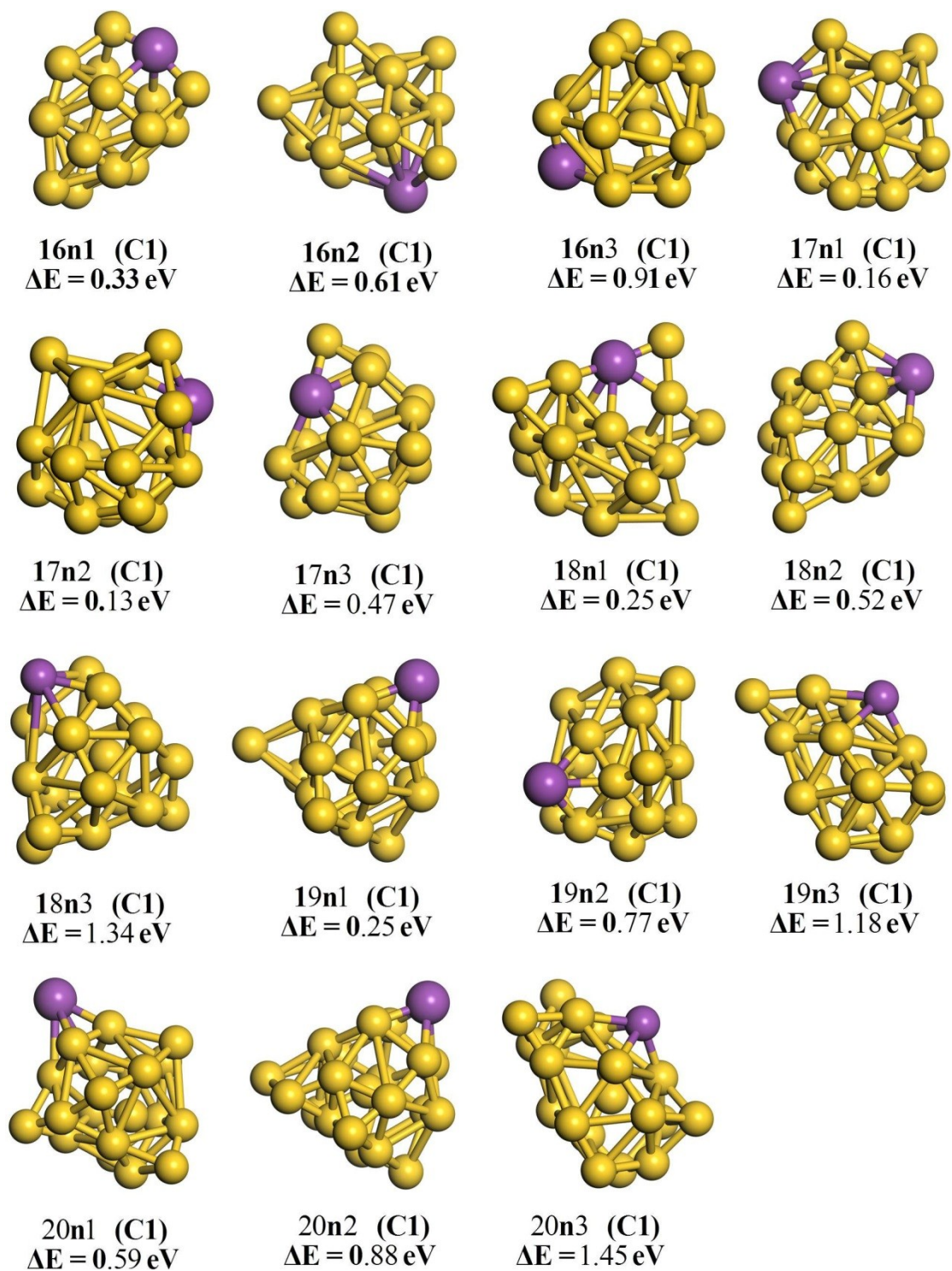


Fig. S3 The metastable structures of the BiAu_n ($n=16-20$) clusters, together with the symmetry and relative energy corresponding to the neutral ground state structures

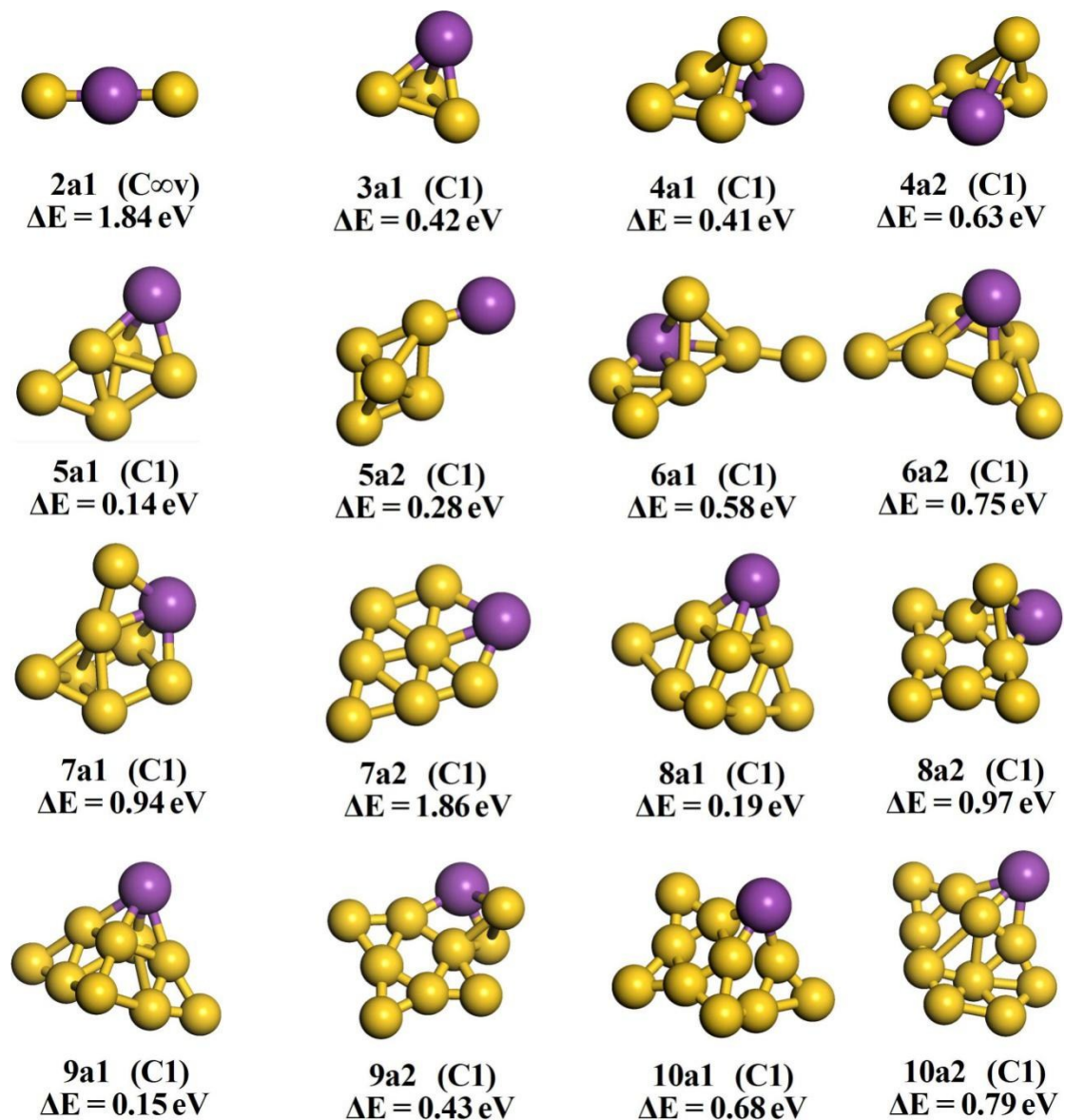


Fig. S4 The metastable structures of the anionic BiAu_n^{-1} ($n=2-10$) clusters, together with the symmetry corresponding to the anionic ground state structures

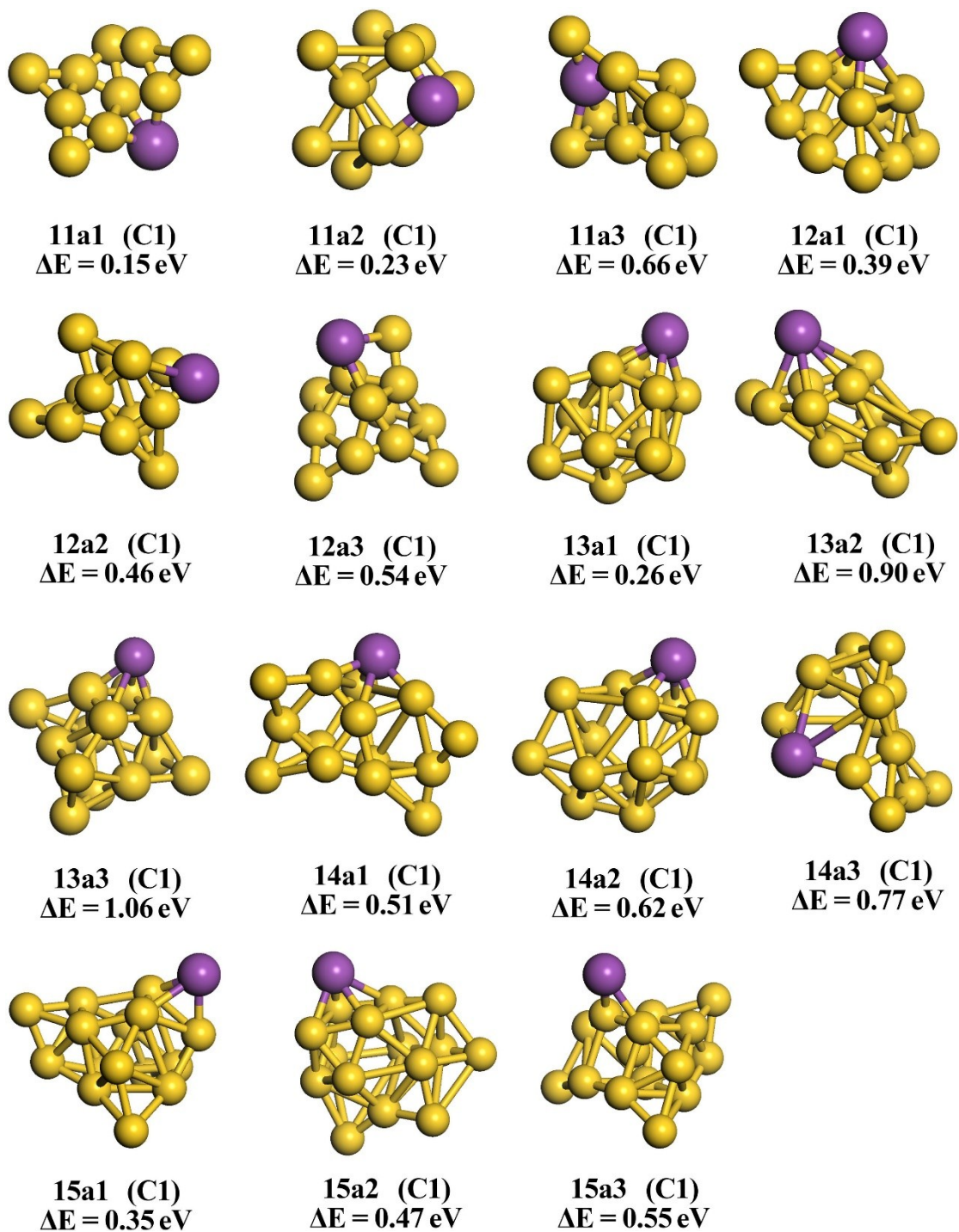


Fig. S5 The metastable structures of the anionic BiAu_n^{-1} ($n=11-15$) clusters, together with the symmetry corresponding to the anionic ground state structures

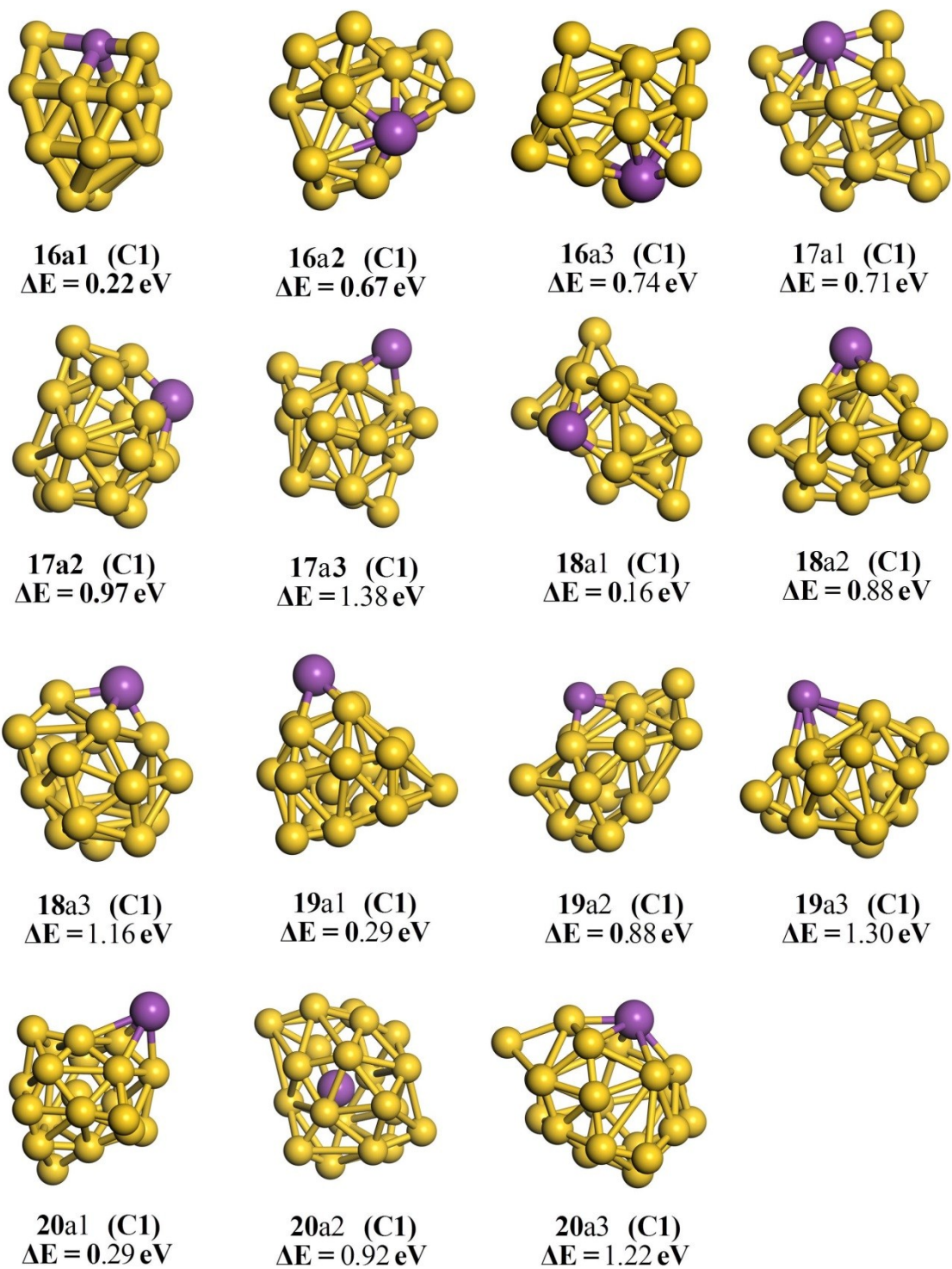


Fig. S6 The metastable structures of the anionic BiAu_n^{-1} ($n=16-20$) clusters, together with the symmetry corresponding to the anionic ground state structures

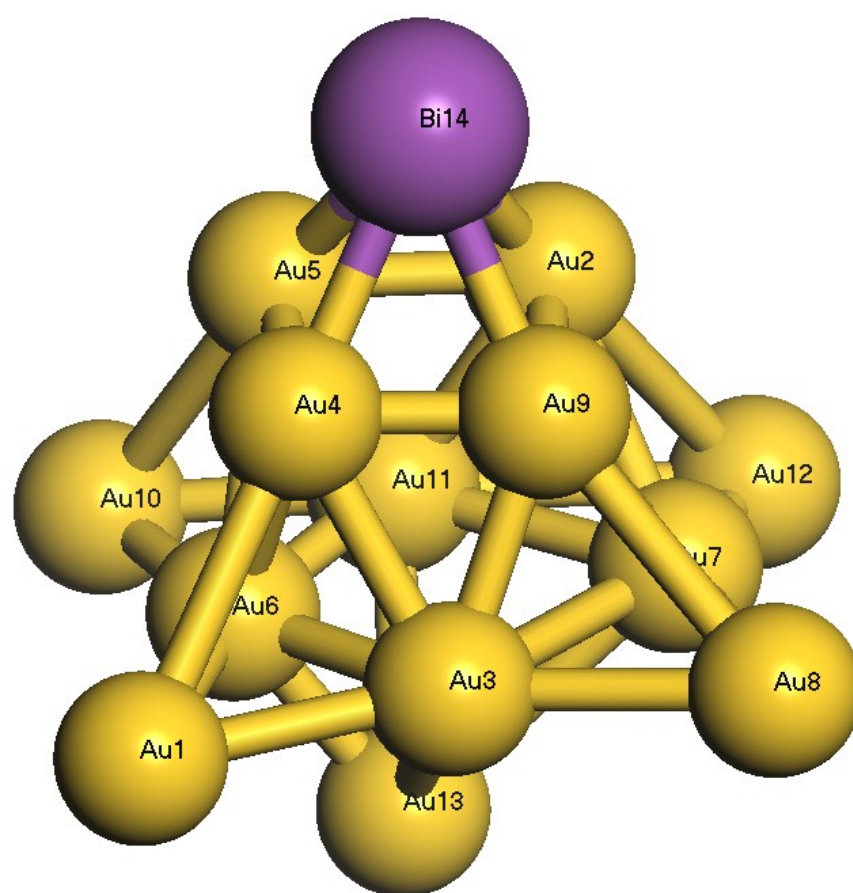


Fig. S7 The molecular graphs of the lowest-energy BiAu₁₃ cluster

Lowest-energy structure of neutral BiAu_n(*n*=2–20) clusters (Coordinates)

BiAu₂

Au	0.00000000	1.81846300	-0.65848800
Au	0.00000000	-1.81846300	-0.65848800
Bi	0.00000000	0.00000000	1.25350700

BiAu₃

Au	0.00000000	2.10031200	-0.41577600
Au	-1.81892400	-1.05015600	-0.41577600
Au	1.81892400	-1.05015600	-0.41577600
Bi	0.00000000	0.00000000	1.18721500

BiAu₄

Au	2.64946200	0.00054000	-0.47114600
Au	0.51764400	-1.63660500	0.19469300
Au	-2.27908700	0.00047800	-1.22436500
Au	0.51645800	1.63673300	0.19606100
Bi	-1.33679100	-0.00109100	1.24187800

BiAu₅

Au	0.79789300	-1.22274200	0.00053800
Au	0.82003700	1.52709700	-0.00077500
Au	-1.42629500	-0.78176100	-1.73657900
Au	3.17843500	-0.03535300	0.00002400
Au	-1.42621200	-0.77981700	1.73747100
Bi	-1.85017800	1.23028300	-0.00064700

BiAu₆

Au	-0.32107800	-0.00143900	1.17946900
Au	-2.43577500	1.39577800	0.11985200
Au	2.37906700	-0.00543200	1.64807900
Au	0.21746400	1.77010000	-0.96789200
Au	0.21337500	-1.76406500	-0.97605500
Au	-2.43739200	-1.39573100	0.11775300
Bi	2.26943200	0.00075100	-1.06717200

BiAu₇

Au	0.37765500	-0.00025800	0.81466600
Au	2.84619300	-0.00133800	-0.26513600
Au	-0.80986500	-1.86739900	-0.92138000
Au	-0.80923300	1.87062500	-0.91664900
Au	-2.23191700	-0.00230600	1.81901100
Au	1.75545000	2.44417500	0.17398300
Au	1.75231200	-2.44542700	0.17398200

Bi	-2.74177100	0.00183500	-0.83614000
BiAu₈			
Au	-1.42645900	1.27313000	-0.35133600
Au	1.36387600	-1.58080600	-0.42931500
Au	1.46191100	1.25374700	-0.35179600
Au	3.26110500	-0.12729600	-1.73930100
Au	-3.26469200	-0.05793000	-1.73692100
Au	-1.40858800	-1.56233700	-0.42505100
Au	0.03133400	3.04629900	1.09155900
Au	0.00911200	0.28582600	2.00176700
Bi	-0.02627000	-2.40867500	1.84688000
BiAu₉			
Au	0.03828300	3.27619700	1.68846700
Au	0.00489700	0.56968700	1.20626400
Au	-3.49482100	-1.41043100	-1.40088500
Au	3.46325900	-1.48750700	-1.39918700
Au	1.43321500	-1.73258200	0.26062300
Au	-0.02110200	-1.93649600	2.54273600
Au	-1.47533600	-1.70159200	0.26417600
Au	-1.88600100	0.80019800	-1.07121200
Au	1.90530400	0.75958400	-1.07053600
Bi	0.03074500	2.72496800	-0.97126800
BiAu₁₀			
Au	3.72834100	2.64373900	-0.61278900
Au	1.36869600	1.69432400	0.31272500
Au	-3.51271800	-0.00056100	-0.48559200
Au	3.51256700	0.00068700	-0.48545400
Au	-1.36901400	-1.69415000	0.31322600
Au	-3.72842100	-2.64362500	-0.61286600
Au	1.36920400	-1.69441900	0.31249300
Au	-1.36952700	1.69401400	0.31351800
Au	-3.73053100	2.64248800	-0.60941200
Au	3.73088300	-2.64230600	-0.60926700
Bi	0.00049400	-0.00018200	2.05915600
BiAu₁₁			
Au	0.00094800	3.33430600	1.19551500
Au	-0.00331400	-2.30443000	-0.52723400
Au	3.73733200	0.30924000	-1.01059700
Au	2.16909800	-1.07014400	0.85900800
Au	1.32851300	-0.43071700	-2.23044900

Au	-1.33203300	-0.43147600	-2.23377100
Au	-3.73671200	0.31403200	-1.00763200
Au	-1.41468200	1.52129700	-0.23483800
Au	1.42116200	1.52193200	-0.23058900
Au	-2.17046400	-1.06605700	0.86226800
Au	0.00049500	0.58450500	2.15917300
Bi	-0.00032700	-2.17248800	2.28352300

BiAu₁₂

Au	-2.66631700	2.62068400	-0.94279900
Au	1.48290300	-1.45486800	1.33075500
Au	-1.96667700	-0.01958500	-1.22481600
Au	-1.48144600	1.45341600	1.33148600
Au	1.45403100	1.48244800	1.33092100
Au	-0.02008700	1.93382800	-1.23149400
Au	0.01916200	-1.93306400	-1.23158900
Au	-2.61273100	-2.67354200	-0.94403300
Au	-1.45331900	-1.48255200	1.33119100
Au	2.61187200	2.67416000	-0.94479700
Au	1.96576500	0.02017700	-1.22446000
Au	2.66539700	-2.62027900	-0.94605600
Bi	0.00137700	-0.00078500	3.20349000

BiAu₁₃

Au	0.00000000	2.06847700	1.53402300
Au	0.00000000	3.76730400	-0.66477700
Au	1.40104000	-1.40104000	-1.00580500
Au	-3.76730400	0.00000000	-0.66477700
Au	3.76730400	0.00000000	-0.66477700
Au	0.00000000	0.00000000	-3.04746200
Au	-2.06847700	0.00000000	1.53402300
Au	0.00000000	-2.06847700	1.53402300
Au	0.00000000	-3.76730400	-0.66477700
Au	-1.40104000	-1.40104000	-1.00580500
Au	1.40104000	1.40104000	-1.00580500
Au	2.06847700	0.00000000	1.53402300
Au	-1.40104000	1.40104000	-1.00580500
Bi	0.00000000	0.00000000	3.42050600

BiAu₁₄

Au	2.00800800	1.48956300	-0.44905100
Au	-2.49757600	0.29301500	2.16095200
Au	1.45253500	-0.80989100	-2.07849600
Au	-3.72054500	-0.68951700	-0.40784600

Au	1.39603300	-1.72388800	0.67967900
Au	-2.01291200	1.48540400	-0.44906700
Au	0.00145700	-0.78073400	2.99347500
Au	-0.00231700	1.53089600	-2.60118600
Au	-1.38680600	-1.72047100	0.67732500
Au	0.00384300	-3.10846100	-1.27818100
Au	-1.45221300	-0.81404700	-2.08033200
Au	2.49590100	0.29952600	2.15848900
Au	-0.00307900	1.63776800	1.62992600
Au	3.72259900	-0.67931600	-0.40950700
Bi	-0.00469100	3.41713300	-0.51986000

BiAu₁₅

Au	2.26639100	0.93946400	0.95761900
Au	-2.90718600	-1.98220400	0.03789400
Au	-0.34963800	-3.17230100	-0.40877400
Au	1.75618100	-1.86834900	1.02768600
Au	-0.30744700	1.62137500	1.81816200
Au	-2.82611900	0.52714900	1.41555300
Au	-1.91608900	2.87839200	-0.05622100
Au	-2.98060900	0.57817000	-1.36072100
Au	-1.30956800	-1.37563600	-2.32975300
Au	1.35969300	-1.31318700	-1.76293400
Au	2.48547800	1.36905400	-1.80342800
Au	0.87806400	3.14792900	-0.33364300
Au	-0.86806200	-1.42280200	1.83607700
Au	-0.30602700	1.15899600	-1.86119000
Au	3.81943700	-0.86452700	-0.63851100
Bi	1.14740500	-0.21084700	3.29533400

BiAu₁₆

Au	0.98898400	2.15402400	-1.52199300
Au	4.14012100	-0.96270400	0.21258900
Au	-1.69834700	2.78916500	-0.99968200
Au	-0.07544600	-2.61947200	-1.49712000
Au	2.72712300	1.33506600	0.61396500
Au	-3.66455200	0.74668000	-1.74728600
Au	-0.84010900	0.15580400	-1.92264100
Au	-2.29031800	0.53265500	0.64514500
Au	1.79230100	3.94622400	0.48066400
Au	-2.71714800	-1.85101800	-1.21820700
Au	1.85681200	-0.47862600	-1.63112600
Au	-0.00165600	1.99255500	1.22317500
Au	-2.92749700	-1.05581300	2.84463700

Au	1.53620000	-1.27140400	1.16951600
Au	-1.06552500	-2.16705800	1.04159900
Au	2.51946400	-3.11607700	-0.82004900
Bi	-0.26689400	-0.12373500	2.97612300

BiAu₁₇

Au	-4.07177000	-2.17715000	-0.29768800
Au	2.44124600	-1.71857600	2.62459200
Au	0.49296500	0.33829600	-1.62046500
Au	3.02910100	1.45273700	-1.16345100
Au	-4.37785900	0.66945400	-0.75394600
Au	1.63926200	0.62994900	1.18424700
Au	-2.65274700	-0.28951500	1.23006700
Au	-0.31356700	-1.02394900	2.38004800
Au	-1.98812300	2.04567500	-0.78529800
Au	0.80785100	2.83255000	-0.40708700
Au	-1.24617600	4.25980200	0.68904100
Au	-0.85506900	1.73005500	1.87037300
Au	-1.39754000	-2.76696900	0.21363500
Au	1.30643900	-2.19332800	0.14611100
Au	-2.11116000	-0.64060700	-1.73624600
Au	3.84124900	-0.91167400	0.31909800
Au	5.44633700	0.24044300	-1.48081000
Bi	0.00909900	-2.35781200	-2.29596900

BiAu₁₈

Au	2.16252700	0.65480400	0.00000000
Au	-2.03329900	-0.41466800	0.00000000
Au	0.54429500	-1.79537200	0.00000000
Au	-1.59354200	-2.91838200	1.40610000
Au	1.97969000	-1.15035900	-2.33092000
Au	1.97969000	-1.15035900	2.33092000
Au	-1.59354200	-2.91838200	-1.40610000
Au	-0.69069600	-0.50973300	2.53754900
Au	-0.69069600	-0.50973300	-2.53754900
Au	1.01183600	0.19048600	-4.65447300
Au	-3.26619200	0.48772200	2.33620000
Au	-3.26619200	0.48772200	-2.33620000
Au	1.01183600	0.19048600	4.65447300
Au	1.28685900	1.74297100	2.43844500
Au	-1.29125800	2.15826300	-1.38010000
Au	-1.29125800	2.15826300	1.38010000
Au	1.28685900	1.74297100	-2.43844500
Au	3.37570400	-1.88790000	0.00000000

Bi	1.02545800	3.27535800	0.00000000
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BiAu₁₉

Au	-0.05678100	2.35710100	-1.73653200
Au	-0.66775100	-0.15908000	-2.33912700
Au	-4.99400200	-1.18352300	0.75973400
Au	-2.41590300	-1.49361200	1.72003300
Au	-0.33987900	-2.12039500	-0.06311000
Au	1.39149900	-2.37432300	-2.19674600
Au	2.63864000	-1.58873100	3.65667400
Au	-2.94008300	-1.10656800	-1.06520900
Au	-1.80040400	3.20920300	0.40103600
Au	-0.60186100	0.64483400	0.82076700
Au	1.82629200	0.77789900	2.49148500
Au	2.94265500	0.99472000	-0.04107900
Au	1.96294200	0.61737900	-2.60270600
Au	0.13978000	4.89449400	-0.63254000
Au	-1.40456800	-2.83652100	-2.61532800
Au	1.14051800	2.89730300	0.97469200
Au	-3.41518100	1.11867900	0.67738200
Au	0.13782300	-1.57707500	2.62849700
Au	2.44803800	-1.77105200	0.81144100
Bi	3.81506000	-1.23804500	-1.56987700

BiAu₂₀

Au	-3.02145300	0.00317400	-1.25077100
Au	3.02021800	-0.00269900	1.25681400
Au	-1.12617900	2.61010600	0.90663400
Au	-1.62853500	-0.01024700	2.46495300
Au	-1.13322400	-2.61202500	0.89549100
Au	1.13537700	-2.61618000	-0.91407800
Au	1.62897100	0.00790200	-2.47126100
Au	1.13533600	2.62228300	-0.91409100
Au	-3.78147800	-1.37099200	1.17478300
Au	-3.01900900	-2.79452100	-1.15790800
Au	-0.86363500	-1.44950900	-2.45634900
Au	-0.86748400	1.45850100	-2.45333400
Au	-3.01714900	2.80076400	-1.14315600
Au	-3.77337600	1.36691600	1.18395800
Au	0.86475900	-1.46523900	2.45665000
Au	3.01721600	-2.79997900	1.14393900
Au	3.77547900	-1.36328900	-1.18123500
Au	3.77794000	1.37283700	-1.17240400
Au	3.00376400	2.79387200	1.15736200

Au	0.86100400	1.44595000	2.47204900
Bi	0.01090500	0.00226200	0.00186200

Lowest-energy structure of anionic BiAu_n⁻¹ (n=2–20) clusters (Coordinates)

BiAu₂⁻¹

Au	0.00000000	1.92506800	-0.63563900
Au	0.00000000	-1.92506800	-0.63563900
Bi	0.00000000	0.00000000	1.21001200

BiAu₃⁻¹

Au	0.00000000	2.61185700	-0.20667600
Au	-2.26193500	-1.30592900	-0.20667600
Au	2.26193500	-1.30592900	-0.20667600
Bi	0.00000000	0.00000000	0.59014600

BiAu₄⁻¹

Au	-1.98953800	-1.85766400	-0.58581800
Au	-1.98889700	1.85788600	-0.58577900
Au	1.33173500	-0.00014000	0.27855400
Au	3.90548300	-0.00012900	-0.31968600
Bi	-1.19811800	0.00004600	1.15428400

BiAu₅⁻¹

Au	0.51111600	-1.01122700	-0.55039000
Au	-0.67079500	1.94296700	-0.04979200
Au	1.94322300	1.28871000	0.45801900
Au	3.17146200	-1.14186700	0.14389100
Au	-2.87563600	-0.89532500	1.22912500
Bi	-1.97916000	-0.17442600	-1.17153400

BiAu₆⁻¹

Au	1.94082900	0.00473000	0.17193700
Au	2.18650000	-2.64865200	0.24913900
Au	-3.17217600	-0.00064200	1.41579600
Au	-0.31670700	-1.63460300	-0.44860000
Au	-0.32585400	1.62906600	-0.45380300
Au	2.16908700	2.66001200	0.24617700
Bi	-2.36208000	-0.00943300	-1.12374900

BiAu₇⁻¹

Au	-0.00013500	0.52822100	0.00180800
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Au	-2.70770000	0.37832500	0.00005100
Au	-2.83474300	-2.36319900	-0.00165700
Au	2.83730900	-2.36025000	-0.00179900
Au	2.70738800	0.38099900	0.00006800
Au	1.44779300	2.86069700	-0.00045600
Au	-1.45099400	2.85921200	-0.00070400
Bi	0.00102900	-2.17393200	0.00255900

BiAu₈⁻¹

Au	1.99735600	0.53307800	-0.89212400
Au	-1.99773600	0.53338400	-0.89164100
Au	3.76070400	-1.50440600	-0.49413500
Au	-3.76099500	-1.50450400	-0.49405900
Au	0.00083500	0.34606200	1.24929700
Au	0.00024500	3.10420100	1.45054800
Au	-1.34042600	-1.99310500	0.64811500
Au	1.34017200	-1.99398800	0.64763300
Bi	-0.00014800	2.35979500	-1.16466400

BiAu₉⁻¹

Au	-2.43605000	-1.82694800	0.16008700
Au	2.37091700	1.04617100	-0.48091400
Au	-2.37086500	1.04690500	-0.48047200
Au	2.43499400	-1.82785900	0.15988400
Au	-0.00015600	-0.37523900	-0.17942600
Au	0.00228700	3.06985600	1.66232800
Au	-0.00076900	-3.04521400	0.43341900
Au	4.68745300	-0.33026000	-0.15508400
Au	-4.68800700	-0.32853100	-0.15472800
Bi	0.00018600	2.44721000	-0.91858400

BiAu₁₀⁻¹

Au	-3.49884400	-2.65054200	-0.88565000
Au	-1.44114000	-1.57313300	0.60682200
Au	3.41507600	-0.00059000	-0.69045300
Au	-3.41524400	0.00070900	-0.69047900
Au	1.44113800	1.57318500	0.60700000
Au	3.49865800	2.65067000	-0.88565800
Au	-1.44023700	1.57331800	0.60661900
Au	1.44045600	-1.57358000	0.60679100
Au	3.49657600	-2.65182400	-0.88721400
Au	-3.49650800	2.65194500	-0.88690600
Bi	0.00006300	-0.00015000	2.37868800

BiAu₁₁⁻¹

Au	1.58066500	0.44467800	3.15106000
Au	2.59571100	-0.49419800	0.56724300
Au	-1.93463400	-2.18057200	0.19930800
Au	0.15610200	-1.45747800	1.79323600
Au	1.23731200	0.46504900	-1.85001700
Au	0.06900400	3.97301200	0.29867300
Au	-2.33667600	0.60887200	-0.41214600
Au	0.27717600	1.23523300	0.82744800
Au	-4.41678200	-1.10441100	0.04983400
Au	0.57813900	-2.26727300	-0.79240900
Au	2.95199500	-1.68420200	-2.00304200
Bi	-0.72148200	2.34267500	-1.74103500

BiAu₁₂⁻¹

Au	-2.69508400	2.64684600	-0.84821900
Au	1.48334900	-1.45536500	1.31948100
Au	-1.92211700	-0.01871900	-1.30163900
Au	-1.48108800	1.45259500	1.32124400
Au	1.45423400	1.48166100	1.32003500
Au	-0.01994900	1.88652100	-1.30882600
Au	0.01829800	-1.88486700	-1.30992500
Au	-2.64104200	-2.69969200	-0.85074300
Au	-1.45288300	-1.48285400	1.32044000
Au	2.63950500	2.70145100	-0.85116200
Au	1.92032700	0.02021300	-1.30144600
Au	2.69413400	-2.64595300	-0.85371100
Bi	0.00220600	-0.00174700	3.18329400

BiAu₁₃⁻¹

Au	2.50026500	-0.39623400	1.30679600
Au	-1.46023100	1.76568600	2.38519000
Au	0.96825900	-2.59914400	0.07613000
Au	2.06568900	-0.37263600	-1.58501500
Au	0.84769200	3.61982000	-1.62482400
Au	3.66989300	-2.28120700	-0.38284700
Au	-3.03264500	0.02002100	1.05819100
Au	-1.69278400	0.27465900	-1.45456600
Au	1.31388200	1.57935200	2.76485800
Au	-0.33780400	-0.74076000	1.72064300
Au	0.44086900	1.48821600	0.11467700
Au	-3.99607700	-1.31312500	-1.18201000
Au	-1.67292600	-2.37191300	-0.14421300
Bi	0.36732100	1.26330100	-2.90587800

BiAu₁₄⁻¹

Au	-1.99011100	1.59714600	-0.21007800
Au	2.45985600	-0.61699000	-2.02788700
Au	-1.41878400	0.21980600	2.40442800
Au	3.54093200	-0.48509800	0.72210400
Au	-1.37814300	-2.10458500	0.02602200
Au	1.98972400	1.59731400	-0.21034200
Au	-0.00010800	-1.88670200	-2.52839900
Au	-0.00010500	2.48549200	1.63206700
Au	1.37848600	-2.10440400	0.02559200
Au	0.00057600	-2.22221400	2.38121100
Au	1.41925100	0.22021300	2.40443100
Au	-2.46012100	-0.61742300	-2.02735500
Au	-0.00027700	0.85277800	-2.21069500
Au	-3.54082900	-0.48556200	0.72262900
Bi	-0.00033000	3.37913300	-1.05053700

BiAu₁₅⁻¹

Au	2.36338300	1.01930900	0.90730600
Au	-2.85424600	-1.93862100	0.19181300
Au	-0.32254900	-3.13627500	-0.29234900
Au	1.81715700	-1.78517800	0.96553300
Au	-0.25823100	1.60493300	1.86071600
Au	-2.83880200	0.53887200	1.52067900
Au	-1.93787200	2.75323500	-0.04895500
Au	-3.11167900	0.51745700	-1.37393700
Au	-1.41083400	-1.44368900	-2.24729900
Au	1.28812200	-1.31738500	-1.84735800
Au	2.35135100	1.31940300	-1.91041900
Au	0.82235200	3.09076600	-0.36656500
Au	-0.78517100	-1.33854700	1.96518800
Au	-0.40875400	1.11286900	-1.97571900
Au	3.82950900	-0.82593100	-0.80026500
Bi	1.38608300	-0.16296600	3.28528700

BiAu₁₆⁻¹

Au	-4.59982000	-0.99468900	-1.80597700
Au	-0.42039100	-2.15725500	-0.40279800
Au	-1.99834700	2.54025400	0.48502100
Au	-0.85304400	-1.25574200	2.33676600
Au	-2.56398900	0.87238100	2.74303600
Au	0.12682000	1.44356200	2.08461500
Au	0.86274200	-3.36430500	1.79374300

Au	2.55081300	1.78834500	0.88272500
Au	2.19808300	1.91635900	-1.92888400
Au	1.25976600	-0.71562300	-2.27002000
Au	2.37797400	-2.60024700	-0.54797500
Au	3.76508500	-0.13851200	-0.64400600
Au	-2.49022500	-0.22697200	0.16092400
Au	1.84371900	-0.74940600	1.55724400
Au	0.53656700	3.42848900	-0.19244100
Au	-0.59772300	1.29904600	-1.66430000
Bi	-1.90173800	-1.03336600	-2.46296600

BiAu₁₇⁻¹

Au	-4.78137200	-1.83500600	0.05781500
Au	2.11066000	-2.16460500	2.49367200
Au	1.31381000	0.15780500	-1.66391300
Au	3.46547600	1.51319700	-0.55423000
Au	-3.68578900	0.50306000	-0.92907500
Au	1.63270700	0.43141700	1.37341000
Au	-2.87791600	-0.58686900	1.61564200
Au	-0.42574700	-1.07235300	2.58740200
Au	-1.96321100	2.57049700	-0.88813100
Au	1.01032800	2.65163700	-0.22849200
Au	-0.83637800	4.26465700	0.97594600
Au	-1.03993500	1.49937900	1.61602700
Au	-2.07661500	-2.10715800	-0.68568500
Au	0.62589400	-2.26515500	0.12766300
Au	-1.35415200	0.30226200	-2.36865900
Au	3.26783700	-1.40944900	-0.09221200
Au	5.59830700	-0.19054900	-0.74671000
Bi	0.01531900	-2.15372100	-2.56080900

BiAu₁₈⁻¹

Au	0.87482600	-1.13194100	1.79946100
Au	1.53009700	-2.78444600	-0.44870100
Au	0.73460500	2.28476400	1.54025500
Au	-1.23947700	2.83593200	-0.39144500
Au	-0.26786200	-0.75858000	-2.06227600
Au	-5.54192100	-0.18633000	-0.82941600
Au	0.94991400	1.70743500	-1.99324700
Au	-1.77088100	-1.82157400	2.78031200
Au	3.58231800	-0.93019400	0.64990200
Au	-3.57823200	1.53630900	-0.11951500
Au	2.48962700	-0.51925400	-2.02374600
Au	-1.06625500	-2.31612100	0.08372700

Au	3.01003700	1.75036600	-0.00603700
Au	-1.40551400	0.56603200	1.34060700
Au	4.19229400	-2.63462500	-1.41352700
Au	-2.93522800	-1.24981700	-1.87362700
Au	1.20368900	4.10708800	-0.69682800
Au	-3.60213100	-1.24442200	0.82497100
Bi	2.70322100	0.75133700	2.70230400

BiAu₁₉⁻¹

Au	-0.09483500	2.34156700	-1.94767900
Au	-1.23693200	-0.09893000	-2.05157800
Au	-4.83038800	-1.29206600	1.44927500
Au	-2.10482700	-1.52669400	1.72532800
Au	0.00740100	-2.08158800	-0.01437400
Au	1.41266500	-2.69736800	-2.30752200
Au	2.91998900	-1.07501600	3.72507500
Au	-3.30900800	-1.49551700	-0.89999500
Au	-1.89003900	3.11661900	0.24282900
Au	-0.47471200	0.69081200	0.75441600
Au	2.00548700	1.09477100	2.29323700
Au	2.74809400	1.06828700	-0.39668300
Au	1.46457200	0.18311200	-2.67195500
Au	-0.13775900	4.94362700	-0.89796100
Au	-1.37216000	-2.91970500	-2.29600300
Au	1.09927500	3.07202600	0.69752400
Au	-3.33905500	0.95976500	0.78819000
Au	0.43458200	-1.35158000	2.65231300
Au	2.77358300	-1.58259900	0.90717300
Bi	3.73495500	-1.28448600	-1.66719600

BiAu₂₀⁻¹

Au	0.54202100	-0.53610500	0.51734700
Au	-0.56941900	2.09591200	-0.18344000
Au	-0.91203900	0.97366700	2.37965400
Au	2.26594400	1.83543500	-1.19286400
Au	-1.51441600	-1.86531300	-1.58243200
Au	2.82420800	-2.23411800	1.02626900
Au	-3.34493600	1.13251600	0.72678100
Au	-2.25134500	3.40200200	1.75721900
Au	-2.56707500	0.84823500	-2.07703100
Au	0.76962700	-3.28535800	-0.64935400
Au	0.21007900	-3.02558200	1.98630000
Au	3.92374500	0.18172300	0.69196800
Au	2.56649600	-0.94886500	-1.54795200

Au	0.28667000	0.37319100	-2.40021700
Au	-2.19170200	-1.56889600	1.26210600
Au	1.64959000	1.76387200	1.67131500
Au	0.66021500	-2.39023300	-3.25133600
Au	-1.11425100	-1.42748700	3.81476900
Au	3.96176400	2.95126800	0.70366200
Au	-0.92836000	2.88908900	-2.85328900
Bi	-4.06118500	-1.10880900	-0.76094600