

SUPPLEMENTARY INFORMATION

Figure S1: Optimized Structures of Isomers 1-6 for Au₁₈, Au₁₉, and Au₂₀ Neutral Cage Clusters.

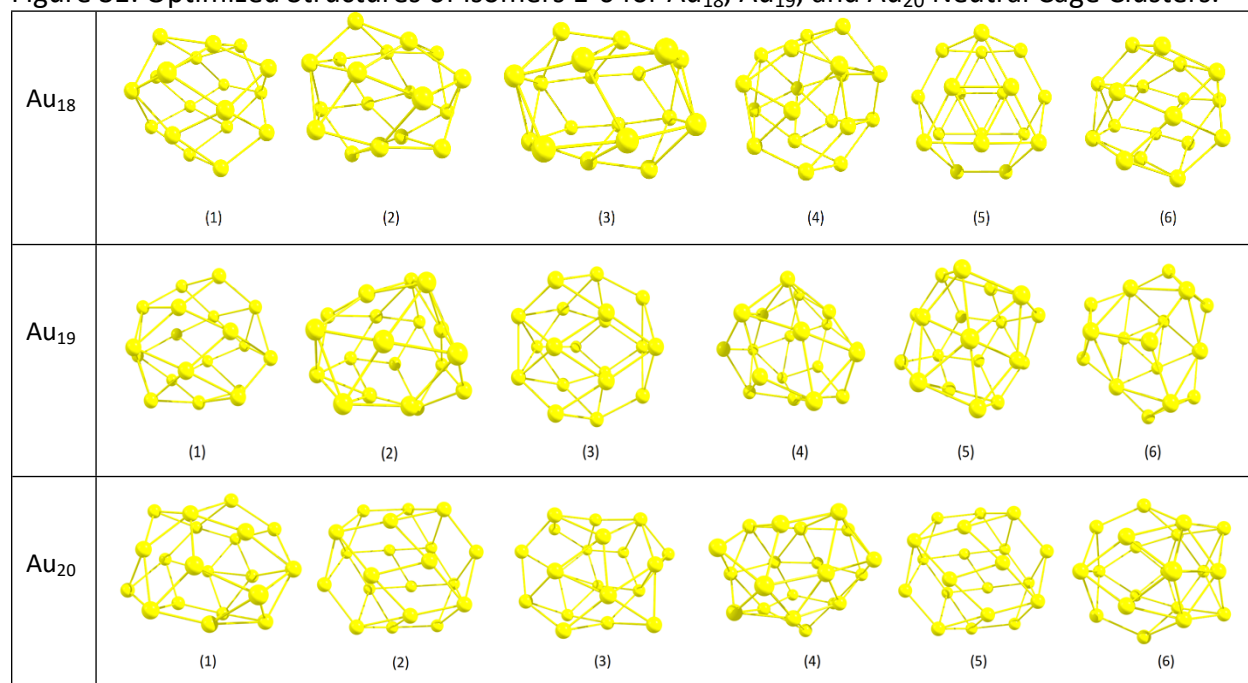


Table S1: Structural Energy (au) Parameters for neutral Au₁₈, Au₁₉, and Au₂₀ Cage and Compact Structures.

	Au ₁₈ ⁰ Cage Energy (au)	Au ₁₈ ⁰ Compact Energy (au)
18:1	-598.1152	-598.1112
18:2	-598.1035	
18:3	-598.0932	
18:4	-598.1236	
18:5	-598.1129	
18:6	-598.1186	
Average	-598.1112	
	Au ₁₉ ⁰ Cage Energy (au)	Au ₁₉ ⁰ Compact Energy (au)
19:1	-631.3362	-631.3599
19:2	-631.3418	
19:3	-631.3396	
19:4	-631.3453	
19:5	-631.3468	
19:6	-631.3475	
Average	-631.3429	
	Au ₂₀ ⁰ Cage Energy (au)	Au ₂₀ ⁰ Compact Energy (au)
20:1	-664.5817	-664.6210
20:2	-664.5810	
20:3	-664.5923	
20:4	-664.5821	

20:5	-664.5810
20:6	-664.5896
Average	-664.5846

Table S2: Spherical Aromaticity Parameters for Au₁₈, Au₁₉, and Au₂₀ Neutral Cage Isomers.

Isomer	Symmetry	NICS (ppm)	HL Gap (eV)
18:1	<i>C</i> ₂	-51.66	1.19
18:2	<i>D</i> ₂	-52.02	1.02
18:3	<i>D</i> _{3d}	-54.70	0.87
18:4	<i>C</i> ₂	-51.15	1.33
18:5	<i>D</i> _{3h}	-47.33	1.10
18:6	<i>D</i> ₃	-56.31	1.26
	Average	-52.20	1.13
19:1	<i>C</i> ₂	+1.15	0.79
19:2	<i>C</i> _s	+11.71	1.25
19:3	<i>C</i> _s	+64.95	0.88
19:4	<i>C</i> ₂	-5.65	1.24
19:5	<i>C</i> ₂	-8.18	1.12
19:6	<i>C</i> _{3v}	+13.57	1.00
	Average	+12.93	1.05
20:1	<i>C</i> ₂	-15.84	0.70
20:2	<i>D</i> ₂	+36.04	0.70
20:3	<i>C</i> ₁	-15.82	0.70
20:4	<i>C</i> _s	-16.53	0.75
20:5	<i>D</i> ₂	+35.45	0.32
20:6	<i>D</i> _{2d}	-7.62	0.76
	Average	+2.61	0.66

Table S3: Spherical Aromaticity Parameters for Au₁₉ and Au₂₀ Cationic Cage Isomers.

Isomer	NICS (ppm)	HL Gap (eV)
19 ⁺ :1	-49.34	1.30
19 ⁺ :2	-49.81	1.32
19 ⁺ :3	-49.00	0.95
19 ⁺ :4	-49.34	1.31
19 ⁺ :5	-50.28	1.17
19 ⁺ :6	-49.60	1.06
Average	-49.56	1.19
20 ⁺ :1	-24.56	0.53
20 ⁺ :2	-24.74	0.85
20 ⁺ :3	-29.28	0.67
20 ⁺ :4	-18.21	0.79
20 ⁺ :5	-2.18	0.77
20 ⁺ :6	-24.52	0.69
Average	-20.58	0.71
20 ²⁺ :1	-41.31	1.06
20 ²⁺ :2	-39.49	0.92
20 ²⁺ :3	-39.62	1.40
20 ²⁺ :4	-40.79	1.06
20 ²⁺ :5	-28.52	0.81

20 ²⁺ :6	-39.36	1.08
Average	-38.18	1.06

Table S4: Spherical Aromaticity Parameters for Au₁₉X and Au₂₀X₂ Cage Isomers.

Isomer	NICS (ppm)	HL Gap (eV)
Au ₁₉ F:1	-44.43	1.22
Au ₁₉ F:2	-40.26	1.07
Au ₁₉ F:3	-44.61	0.99
Au ₁₉ F:4	-45.64	1.05
Au ₁₉ F:5	-42.30	1.11
Au ₁₉ F:6	-43.42	1.13
Au ₁₉ Cl:1	-42.81	1.12
Au ₁₉ Cl:2	-36.70	0.89
Au ₁₉ Cl:3	-41.71	0.97
Au ₁₉ Cl:4	-45.18	1.05
Au ₁₉ Cl:5	-43.68	0.93
Au ₁₉ Cl:6	-38.66	0.99
Au ₁₉ Br:1	-41.65	1.09
Au ₁₉ Br:2	-35.16	1.03
Au ₁₉ Br:3	-40.90	0.96
Au ₁₉ Br:4	-41.21	0.97
Au ₁₉ Br:5	-43.20	0.92
Au ₁₉ Br:6	-37.95	0.97
Au ₁₉ I:1	-39.54	1.04
Au ₁₉ I:2	-32.13	0.96
Au ₁₉ I:3	-39.13	0.96
Au ₁₉ I:4	-40.24	0.92
Au ₁₉ I:5	-42.34	0.87
Au ₁₉ I:6	-36.56	0.94
Au ₂₀ F ₂ :1	-31.78	1.16
Au ₂₀ F ₂ :2	-34.09	0.95
Au ₂₀ F ₂ :3	-30.56	1.22
Au ₂₀ F ₂ :4	-34.24	1.02
Au ₂₀ F ₂ :5	-31.58	0.76
Au ₂₀ F ₂ :6	-28.67	0.70
Au ₂₀ Cl ₂ :1	-31.16	1.13
Au ₂₀ Cl ₂ :2	-30.82	0.87
Au ₂₀ Cl ₂ :3	-22.99	0.95
Au ₂₀ Cl ₂ :4	-19.57	0.94
Au ₂₀ Cl ₂ :5	-30.86	0.87
Au ₂₀ Cl ₂ :6	-23.75	0.94
Au ₂₀ Br ₂ :1	-31.06	1.08
Au ₂₀ Br ₂ :2	-31.00	0.86
Au ₂₀ Br ₂ :3	-25.45	0.95
Au ₂₀ Br ₂ :4	-18.93	0.93
Au ₂₀ Br ₂ :5	-28.95	0.83
Au ₂₀ Br ₂ :6	-23.19	0.92
Au ₂₀ I ₂ :1	-33.31	0.67
Au ₂₀ I ₂ :2	-30.15	0.87

$\text{Au}_{20}\text{I}_2:3$	-21.66	0.98
$\text{Au}_{20}\text{I}_2:4$	-17.53	0.90
$\text{Au}_{20}\text{I}_2:5$	-30.14	0.87
$\text{Au}_{20}\text{I}_2:6$	-21.94	0.89

Figure S2: Optimized Structures of Isomer 1: Au_{19}X and Au_{20}X_2 Cage Clusters.

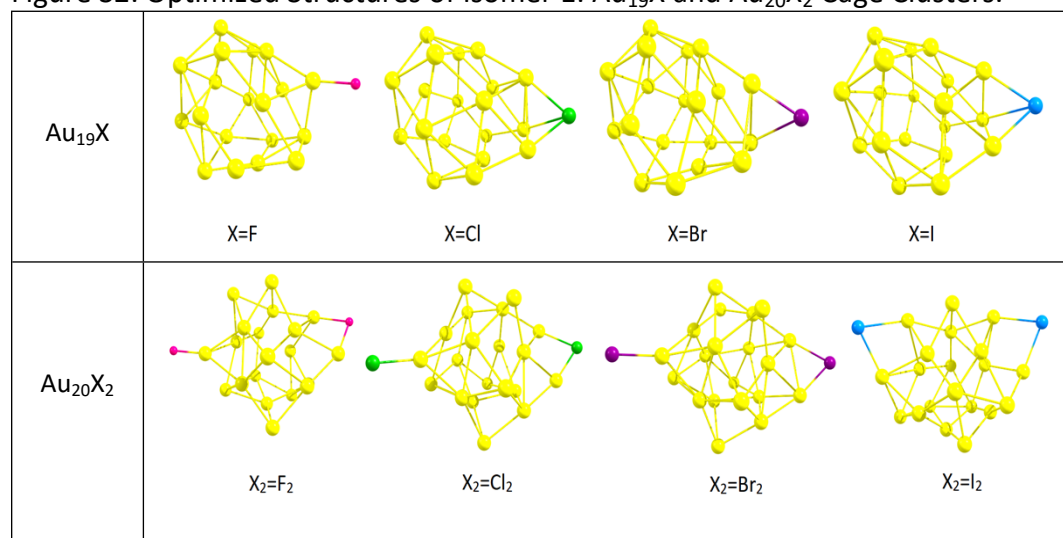


Table S5: Average Spherical Aromaticity Parameters for Au_{19}X and Au_{20}X_2 .

	NICS (ppm)	HL Gap (eV)
Au_{19}F	-43.44	1.10
Au_{19}Cl	-41.46	0.99
Au_{19}Br	-40.01	0.99
Au_{19}I	-38.33	0.95
Au_{20}F_2	-31.82	0.97
$\text{Au}_{20}\text{Cl}_2$	-26.53	0.95
$\text{Au}_{20}\text{Br}_2$	-26.43	0.94
Au_{20}I_2	-25.79	0.86