Bond-bending isomerism and metallophilicity in clusters $(Cu,Ag,Au)_2X_3^-, X = F, Cl, Br, I, At$.

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Supplementary Information

Table I: Structural equilibrium parameters (<Au-X-Au> angle and bond lengths) in $(Au_2X_3)^-, X = F, Cl, Br, I, At$

	Acute angle minima				**Obtuse angle minima**			
	Θ°	d1 (Å)	d2 (Å)	d (Å)	Θ°	d1 (Å)	d2 (Å)	d (Å)
F	-	-	-	-	112.39	2.059	1.958	3.412
Cl	-	-	-	-	102.41	2.313	2.262	3.587
Ma [1]	-	-	-	-	*105.39*	-	-	*3.690*
Br	-	-	-	-	99.99	2.433	2.396	3.743
I	66.27	2.650	2.575	2.909	97.17	2.601	2.572	3.902
Li [2]	*72.00*	*2.620*	*2.560*	*3.080*	*100.70*	*2.590*	*2.560*	*3.990*
At	60.50	2.815	2.707	2.835	94.00	2.732	2.702	3.997

Table II: Bader analysis of acute $(Au_2X_3)^-, X = I, At$ clusters

	λ_1	λ_2	λ_3	$\nabla^2\rho_{(r_c)}$	$\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$
$(Au_2I_3)^-$	-0.0272	-0.0143	0.1166	0.0752	0.0392	0.0255	-0.0412	-0.0157
$(Au_2At_3)^-$	-0.0608	-0.0542	0.1941	0.0791	0.0728	0.0489	-0.0790	-0.0308
$(Ag_2At_3)^-$	-0.0577	-0.0478	0.2148	0.0109	0.0637	0.0310	-0.0460	-0.0151

Table III: Structural equilibrium parameters (<Ag-X-Ag> angle and bond lengths) in $(Ag_2X_3)^-, X = F, Cl, Br, I, At$

	Acute angle minima				**Obtuse angle minima**			
	Θ°	d1 (Å)	d2 (Å)	d (Å)	Θ°	d1 (Å)	d2 (Å)	d (Å)
F	-	-	-	-	115.69	2.096	2.006	3.548
Cl	-	-	-	-	92.14	2.379	2.313	3.427
Br	75.14	2.516	2.444	3.068	-	-	-	-
I	67.77	2.691	2.620	2.997	-	-	-	-
At	61.94	2.816	2.735	2.899	-	-	-	-

Table IV: Structural equilibrium parameters (<Cu-X-Cu> angle and bond lengths in $(Cu_2X_3)^-, X = F, Cl, Br, I, At$

	Acute angle minima				**Obtuse angle minima**			
	Θ°	d1 (Å)	d2 (Å)	d (Å)	Θ°	d1 (Å)	d2 (Å)	d (Å)
F	95.85	1.870	1.785	2.776	-	-	-	-
Cl	76.18	2.158	2.101	2.667	-	-	-	-
Br	69.15	2.300	2.237	2.610	-	-	-	-
I	61.05	2.492	2.427	2.531	-	-	-	-
At	57.15	2.621	2.539	2.197	-	-	-	-

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