$[M_{16}Ni_{24}(CO)_{40}]^{4-}$: Coinage Metal Tetrahedral Superatoms as Useful Building Blocks Related to Pyramidal Au_{20} cluster (M = Cu, Ag, Au). Electronic and Bonding Properties from Relativistic DFT Calculations

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Content:

	E_c (kcal/mol)	ΔE_{H-L} (eV)	M-M (Å)	M-M’ (Å)	M’-M’ (Å)		Lowest freq. (cm^{-1})
$[Cu_{16}]^{4-}$	-56.05	1.52	2.671	2.444	2.424-2.454		69 (t_2)
$[Ag_{16}]^{4-}$	-53.18	1.40	3.023	2.820	2.806-2.828		44 (t_2)
$[Au_{16}]^{4-}$	-46.99	0.65	3.911	2.831	2.737-2.738		35 (t_2)
T_d	$[M_{20}]$ / **$1S^2$ $1P^6$ $1D^{10}$ $2S^2$**						
	E_c (kcal/mol)	ΔE_{H-L} (eV)	M-M (Å)	M-M’ (Å)	M’-M’ (Å)	M’-M’’ (Å)	Lowest freq. (cm^{-1})
$[Cu_{20}]$	-62.07	1.34	2.600	2.453	2.414-2.489	2.390	67 (t_1)
$[Ag_{20}]$	-45.46	1.64	3.034	2.831	2.755-2.902	2.756	41 (t_1)
$[Au_{20}]$	-56.34	1.81	3.131	2.817	2.674-2.946	2.710	30 (t_1)

Table S1. Relevant computed data for $[M_{16}]^{4-}$ and $[M_{20}]$ clusters (M=Cu, Ag, Au) of jellium configuration $1S^2$ $1P^6$ $1D^{10}$ $2S^2$.

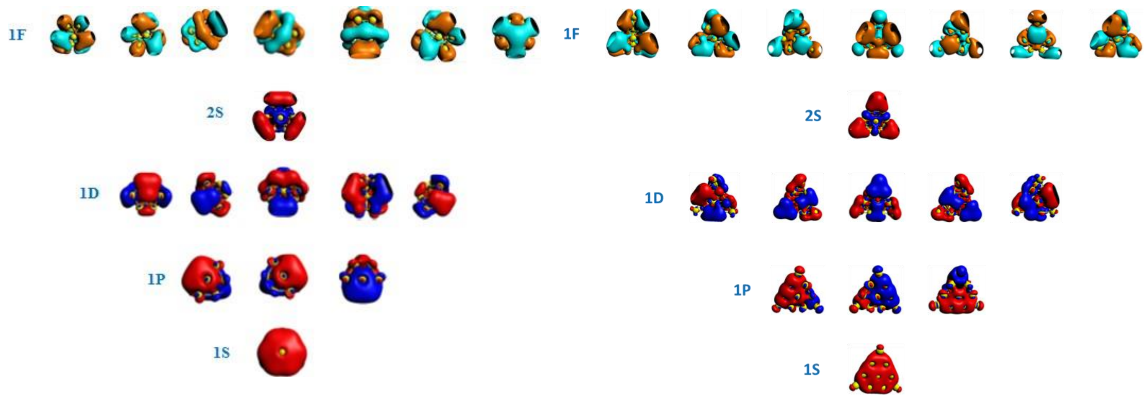

Figure S1. The Kohn-Sham jellium orbitals of $[Au_{16}]^{4-}$ and $[Au_{20}]$

Table S2. Major electronic absorption for $[M_{16}Ni_{24}(CO)_{40}]^{4-}$ (M = Cu, Ag, Au) computed at the PBE and BP86 levels. Oscillator strengths are given in parenthesis.

Copper		Silver		Gold	
PBE	BP86	PBE	BP86	PBE	BP86
1.66 (0.08)	1.66 (0.08)	1.70 (0.13)	1.70 (0.05)	1.64 (0.08)	1.64 (0.02)
1.94 (0.03)	1.97 (0.03)	2.02 (0.11)	2.03 (0.02)	2.01 (0.04)	2.01 (0.02)