Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Electronic Supporting Information file for:

Y@Cu_{15}. A Novel Spherical Aromatic 18-*ce* Bare Superatomic Molecular Cluster

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Content

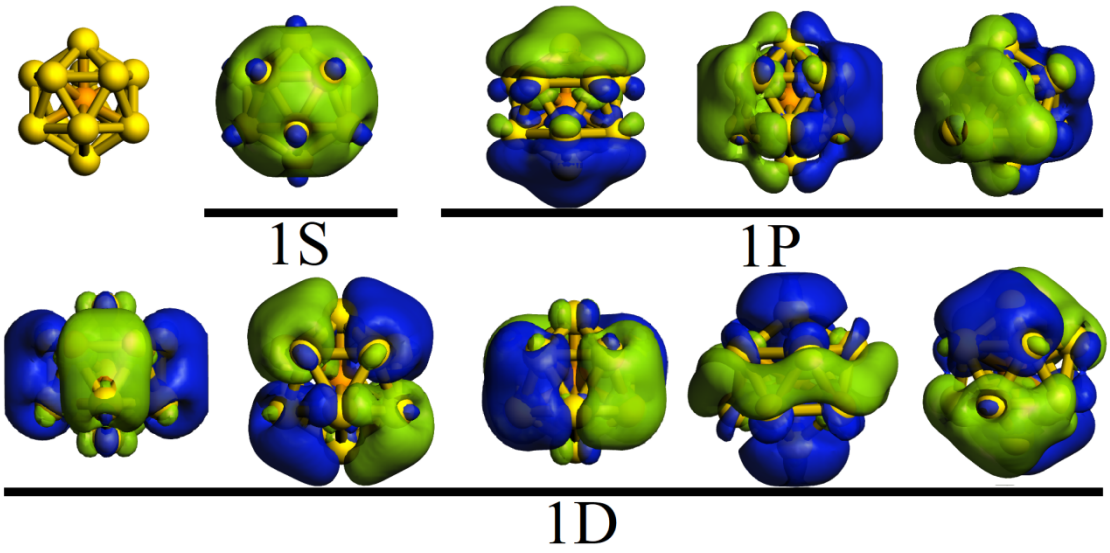

Figure S1. Superatomic orbitals for the W@Au_{12} cluster, denoting a $1S^21P^61D^{10}$ electronic shells structure.

Table S1. Energy decomposition analysis for the Y^{3+}-Cu_{15}^{3-} and W^{3+}-Au_{12}^{3-} interaction. Values in kcal/mol.

	Y@Cu_{15}		W@Au_{12}	
ΔE_{Pauli}	405.9		544.0	
ΔE_{elstat}	-864.9	55.7%[a]	-889.4	43.7%[a]
ΔE_{orb}	-679.2	43.7%[a]	-1135.0	55.8%[a]
ΔE_{disp}	-9.0	0.6%[a]	-9.1	0.4%[a]
ΔE_{int}	-1147.3		-1489.5	
$\Delta\rho_1$	-104.7	15.4%[b]	-149.8	13.2%[b]
$\Delta\rho_1$	-100.5	14.8%[b]	-131.6	11.6%[b]
$\Delta\rho_3$	-98.4	14.5%[b]	-104.0	9.2%[b]
$\Delta\rho_4$	-96.0	14.1%[b]	-97.1	8.6%[b]
$\Delta\rho_5$	-91.5	13.5%[b]	-91.7	8.1%[b]
$\Delta\rho_6$	-16.4	2.4%[b]		

[a]Percentage contribution to stabilizing terms. [b]Percentage contribution to ΔE_{orb} term.

Table S2. Optimized coordinates for the studied species in a MultiXYZ format. Values in Angstrom (Å).

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16
Y@Cu15
Cu       2.094900162      1.326400100      1.018164211
Cu       0.000000000      1.215400092      2.502864325
Cu      -2.094900162      1.326400100      1.018164211
Cu       0.000000000      2.720800207      0.599364181
Cu      -2.094900162     -1.326400100      1.018164211
Cu       2.094900162     -1.326400100      1.018164211
Cu      -1.229300096      1.990700151     -1.410335973
Cu       1.229300096      1.990700151     -1.410335973
Cu       0.000000000     -1.215400092      2.502864325
Cu       2.527500193      0.000000000     -1.074335947
Cu       0.000000000     -2.720800207      0.599364181
Cu      -2.527500193      0.000000000     -1.074335947
Cu      -1.229300096     -1.990700151     -1.410335973
Cu       0.000000000      0.000000000     -2.559536059
Cu       1.229300096     -1.990700151     -1.410335973
Y        0.000000000      0.000000000      0.053864139
13
W@Au12
W        0.000000000      0.000000000      0.000000000
Au       0.000000000      2.452382530      1.223394298
Au      -2.332354546     -0.757827859     -1.223394298
Au       2.332354546      0.757827859      1.223394298
Au       0.000000000     -2.452382530     -1.223394298
Au      -1.441474593      1.984019388     -1.223394298
Au       2.332354546     -0.757827859     -1.223394298
Au      -2.332354546      0.757827859      1.223394298
Au       1.441474593     -1.984019388      1.223394298
Au       1.441474593      1.984019388     -1.223394298
Au       0.000000000      0.000000000      2.739801448
Au       0.000000000      0.000000000     -2.739801448
Au      -1.441474593     -1.984019388      1.223394298
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