

Supporting information for:

Cuboctahedral Pd₁₃ as a spherical Aromatic Noble Metal Core. Insights from ligand-protected [Pd₁₃(Tr)₆]²⁺ Cluster

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Figure S1. Complete description of density deformation channels, $\Delta\rho$, for the Pd-[Pd₁₂(Tr)₆]²⁺ interaction. Density flow from red to blue isosurfaces. Isosurface value set at 0.001 a.u..

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Table S1. Energy decomposition analysis for $\text{Tr}^+ - [\text{Pd}_{12}(\text{Tr})_5]^+$ interaction. Values in kcal/mol.

ΔE_{Pauli}	404.4	
ΔE_{elstat}	-198.2	42.6%
ΔE_{orb}	-248.2	53.3%
ΔE_{disp}	-19.0	4.1%
ΔE_{int}	-61.0	
$\Delta \rho_1$	-80.5	32.4%
$\Delta \rho_2$	-66.1	26.6%
$\Delta \rho_3$	-13.4	5.4%
$\Delta \rho_4$	-10.4	4.2%

Table S2. Energy decomposition analysis for $\text{Pd} - [\text{Pd}_{12}(\text{Tr})_6]^{2+}$ interaction. Values in kcal/mol.

ΔE_{Pauli}	429.6	
ΔE_{elstat}	-432.6	77.6%
ΔE_{orb}	-108.4	19.4%
ΔE_{disp}	-16.4	2.9%
ΔE_{int}	-127.8	
$\Delta \rho_1$	-17.0	15.7%
$\Delta \rho_2$	-14.9	13.8%
$\Delta \rho_3$	-16.1	14.8%
$\Delta \rho_4$	-15.5	14.3%
$\Delta \rho_5$	-15.1	13.9%
$\Delta \rho_6$	-9.3	8.6%
$\Delta \rho_7$	-3.0	2.8%
$\Delta \rho_8$	-3.0	2.8%
$\Delta \rho_9$	-3.0	2.8%

Table S3. Energy decomposition analysis for $\text{Tr}^+[\text{Pd}_{12}(\text{Tr})_5]^+$, $\text{Bz}[\text{Pd}_{12}(\text{Tr})_5]^+$, $\text{Tr}^+[\text{Pd}_{12}(\text{Bz})_5]^+$, and $\text{Bz}[\text{Pd}_{12}(\text{Bz})_5]^+$ interaction. Values in kcal/mol.

	$\text{Tr}^+[\text{Pd}_{12}(\text{Tr})_5]^+$		$\text{Bz}[\text{Pd}_{12}(\text{Tr})_5]^+$		$\text{Tr}^+[\text{Pd}_{12}(\text{Bz})_5]^+$		$\text{Bz}[\text{Pd}_{12}(\text{Bz})_5]^+$	
ΔE_{Pauli}	404.4		356.5		647.1		527.7	
ΔE_{elstat}	-198.2	42.6%	-245.1	60.2%	-641.4	62.6%	-349.0	62.1%
ΔE_{orb}	-248.2	53.3%	-145.3	35.7%	-364.8	35.6%	-197.3	35.1%
ΔE_{disp}	-19.0	4.1%	-16.8	4.1%	-18.2	1.8%	-15.9	2.8%
ΔE_{int}	-61.0		-50.7		-377.4		-34.4	

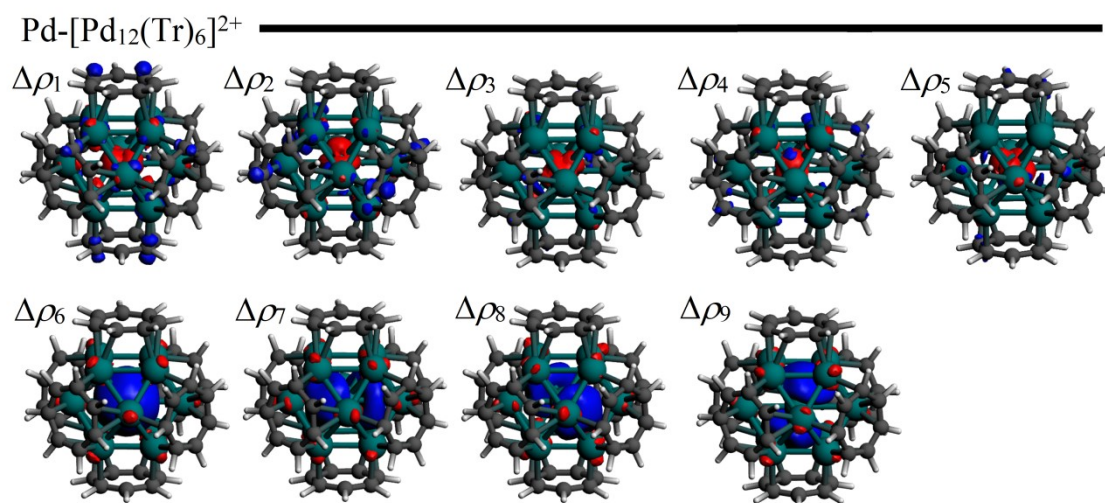


Figure S1. Complete description of density deformation channels, $\Delta\rho_i$, for the $\text{Pd}[\text{Pd}_{12}(\text{Tr})_6]^{2+}$ interaction. Density flow from red to blue isosurfaces. Isosurface value set at 0.001 a.u..