SUPPORTING INFORMATION FOR:

Heavy Elements Metallacycles: Insights into the Nature of Host-Guest Interactions involving Di-Halide Mercuramacrocycle Complexes

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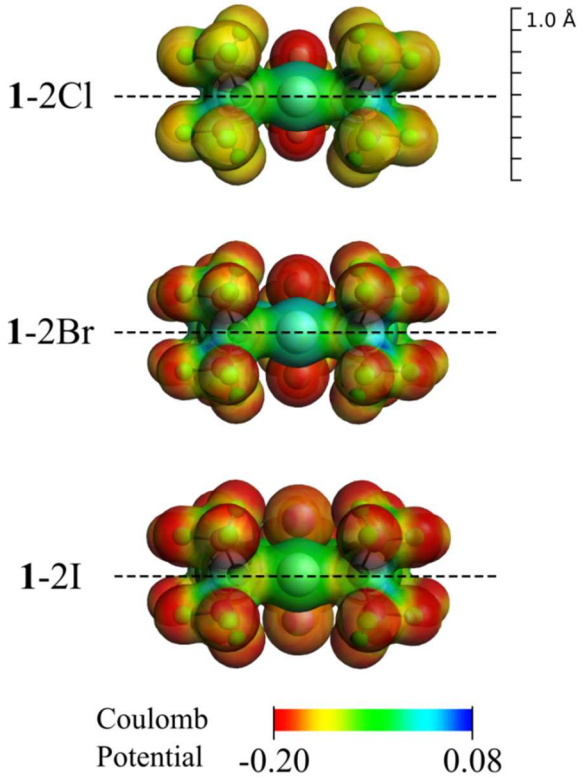

Figure S1. Electrostatic potential map for the studied host-guest systems.

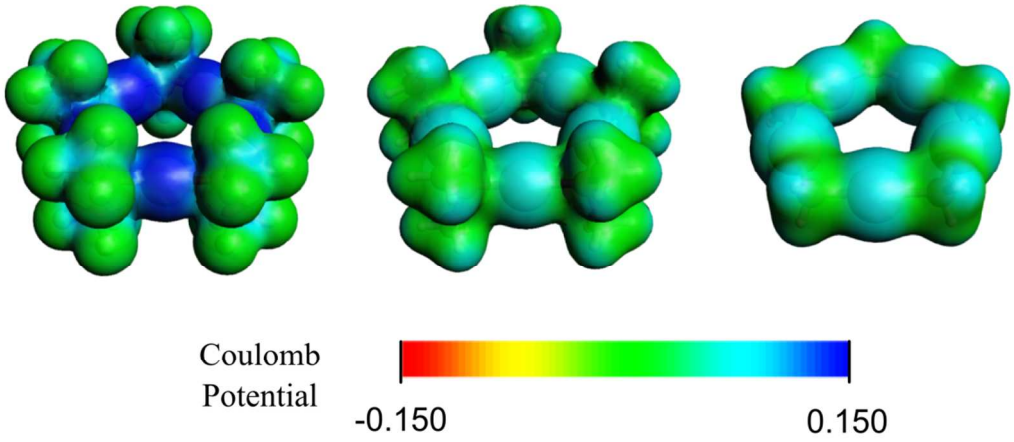

Figure S2. Electrostatic potential map for -CF_3, -CH_3 and -H hosts, respectively.

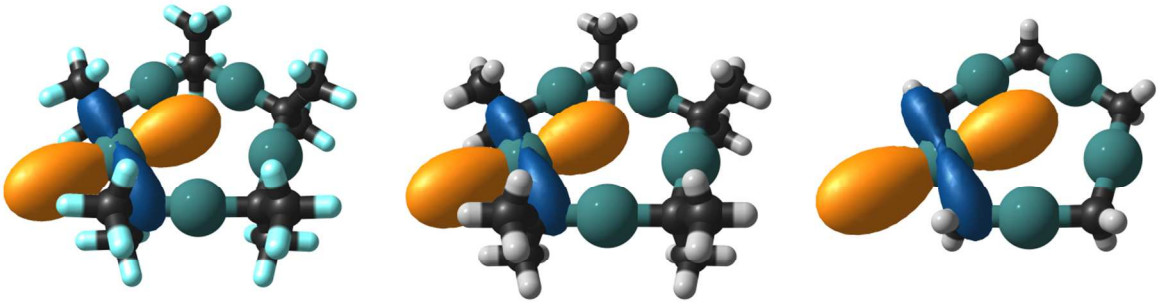

Figure S3. Representative quadrupole tensor denoting its angular dependence for -CF_3, -CH_3 and -H hosts, respectively.

Table S1. Selected calculated distances (Å) and angles (degrees) for the hypothetical **1**-Cl, **1**-Br and **1**-I guest-centered mercuramacrocycle complexes.

	$[(HgC(CF_3)_2)_5X]^-$, X = Cl, Br, I		
	1-Cl	**1**-Br	**1**-I
Hg-Hg	3.531	3.569	3.654
Hg-C	2.189	2.201	2.229
< Hg-C-Hg	107.6	108.3	110.1
< C-Hg-C	180.5	180.4	180.1
Hg···X	3.001	3.038	3.108

Table S2. Selected calculated distances (Å) and angles (degrees) for the hypothetical **1**-Cl, **1**-Br and **1**-I guest-apical mercuramacrocycle complexes.

	$[(HgC(CF_3)_2)_5X]^-$, X = Cl, Br, I		
	1-Cl	**1**-Br	**1**-I
Hg-Hg	3.495	3.490	3.507
Hg-C	2.180	2.177	2.181
< Hg-C-Hg	106.6	106.5	107.0
< C-Hg-C	182.5	183.5	184.3
Hg···X	3.084	3.226	3.435
X···center	0.819	1.126	1.702

Table S3. Energy Decomposition Analysis under the PBE/TZP level for the studied systems (kcal/mol).

$[(HgC(CF_3)_2)_5X_2]^{2-}$, X = Cl, Br, I						
EDA	**1**-2Cl		**1**-2Br		**1**-2I	
ΔE_{orb}	-84.65	33.42%	-85.06	31.27%	-82.52	28.93%
ΔE_{elec}	-161.02	63.56%	-177.92	65.40%	-189.72	66.52%
ΔE_{disp}	-7.65	3.02%	-9.06	3.33%	-12.98	4.55%
ΔE_{Pauli}	72.29		103.78		133.75	
ΔE_{int}	-181.03		-168.26		-151.47	

Table S4. Selected calculated distances (Å) and angles (degrees) for the hypothetical **1**-2Ar, **1**-2Kr and **1**-2Xe mercuramacrocycle complexes.

	$[(HgC(CF_3)_2)_5Ng_2]$, Ng = Ar, Kr, Xe		
	1-2Ar	**1**-2Kr	**1**-2Xe
Hg-Hg	3.546	3.543	3.547
Hg-C	2.168	2.169	2.169
< Hg-C-Hg	109.7	109.6	109.7
< C-Hg-C	181.7	181.6	181.7
Hg···Ng	3.764	3.841	4.031
Ng···center	2.252	2.390	2.674
Ng···Ng	4.504	4.779	5.347

Table S5: Energy Decomposition Analysis of the hypothetical noble-gas complexes (kcal/mol).

$[(HgC(CF_3)_2)_5Ng_2]$, Ng = Ar, Kr, Xe						
	1-2Ar		**1**-2Kr		**1**-2Xe	
ΔE_{orb}	-4.68	22.55%	-5.28	19.24%	-7.20	20.61%
ΔE_{elec}	-4.29	20.67%	-6.87	25.04%	-9.35	26.76%
ΔE_{disp}	-11.78	56.77%	-15.29	55.72%	-18.39	52.63%
ΔE_{Pauli}	9.21		15.89		23.37	
ΔE_{int}	-11.54		-11.55		-11.57	