Supplementary information

How many electrons to stabilize the icosahedral Cu_{55} core in ligated nanoclusters? The example of $[Cu_{55}(NHC)_6]$

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Table S1. Selected metrical data for the open-shell neutral $[Cu_{55}(NHC^B)_6]$ (55 electrons) and thiolate-protected $[Cu_{55}(SH)_6]^-$ (50 electrons) models. All distances (in Å) are averaged to I_h symmetry.

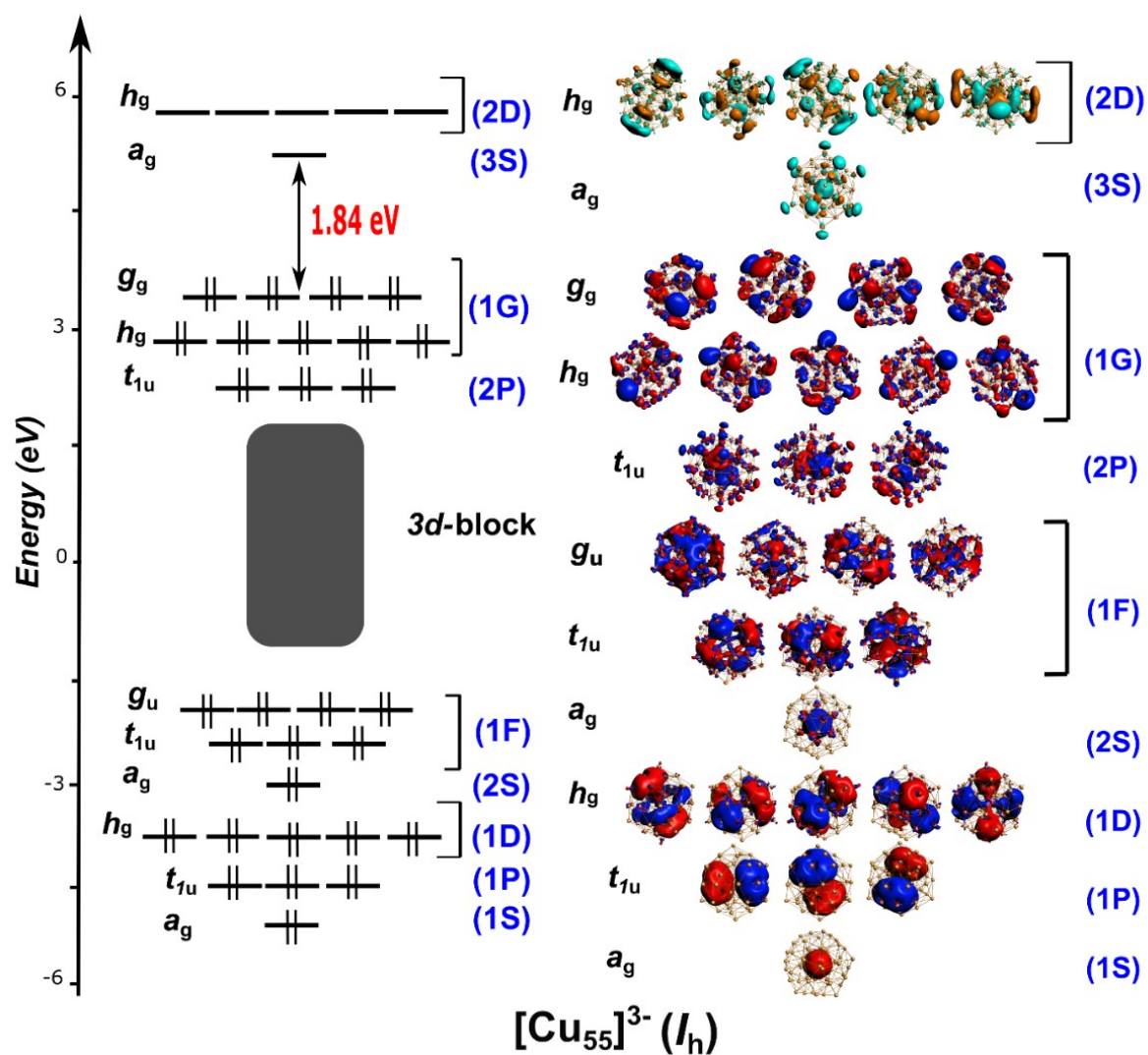|	$[Cu_{55}(NHC^B)_6]$	$[Cu_{55}(SH)_6]^-$
Superatomic electron count	55	50
Symmetry	T_h	T_h
1G splitting/occupation	$t_g^6 e_g^4 t_g^5$	$t_g^6 e_g^4 t_g^0$
HOMO-LUMO gap (eV)	-	2.06
Cu(1)-Cu(2)	2.433	2.440
Cu(2)-Cu(2)	2.572	2.561
Cu(2)-Cu(3)	2.555	2.520
Cu(2)-Cu(4)	2.409	2.454
Cu(3)-Cu(3)	2.642	2.630
Cu(3)-Cu(4)	2.578	2.574
Cu-C/Cu-S	1.979	2.232
Cu...C	2.885	-

Figure S1. Kohn-Sham orbital level ordering of the hypothetical 58-electron $[Cu_{55}]^{3-}$ cluster. The superatomic orbitals are plotted on the right side.
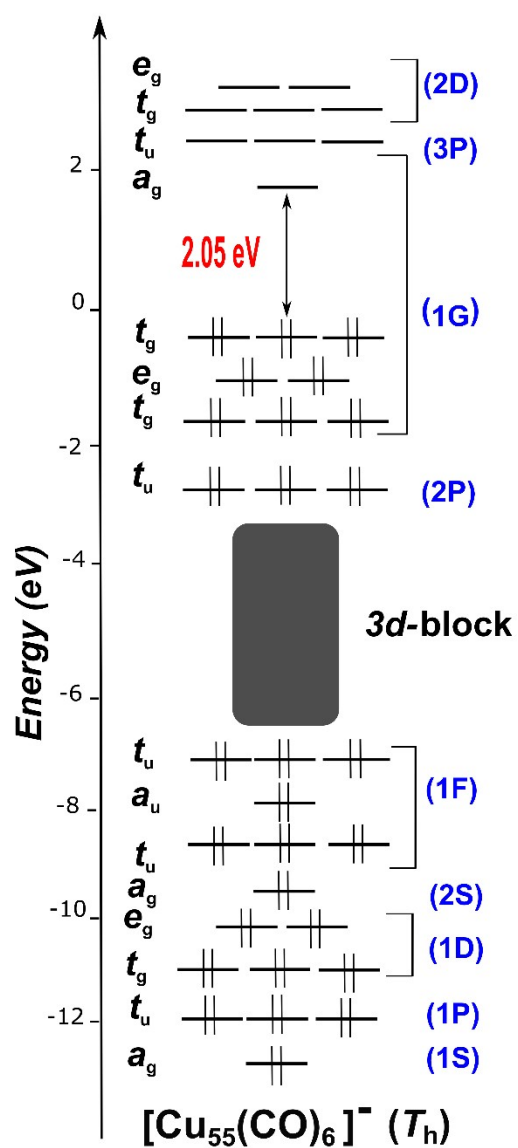
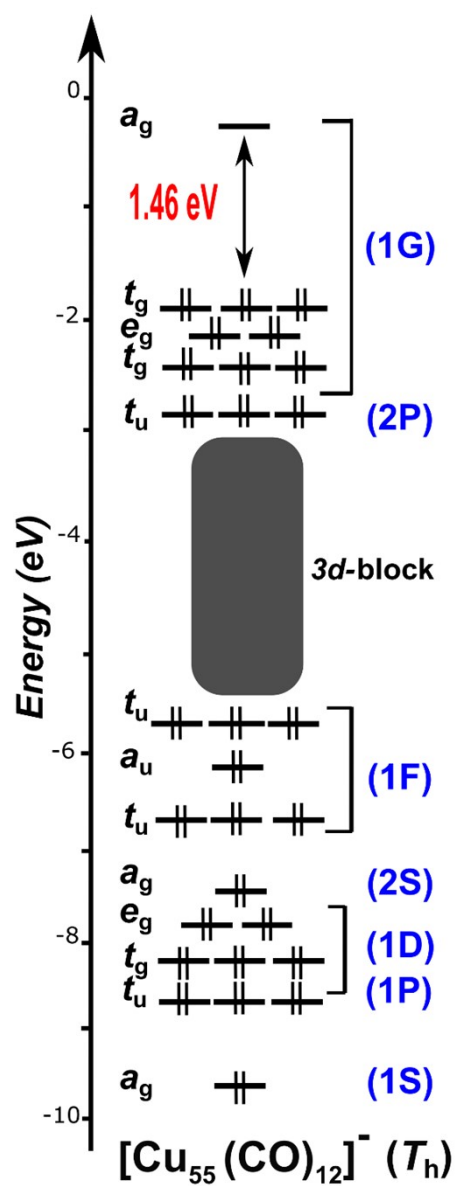**Figure S2**. Kohn-Sham orbital diagram of the 56-electron $[Cu_{55}(CO)_6]^-$ model cluster.

Figure S3. Kohn-Sham orbital diagram of the 56-electron $[Cu_{55}(CO)_{12}]^-$ model cluster.