Evidence of hollow golden cages: Supplementary Materials and Supporting Information

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Fig. 3.  Simulated anion photoelectron spectra [based on the density-functional theory (DFT) calculation with the PBE0/LANL2DZ functional and basis set] for all of the candidate lowest-energy isomers of $\text{Au}_{15}$ ($A$), $\text{Au}_{16}$ ($B$), $\text{Au}_{17}$ ($C$), and $\text{Au}_{18}$ ($D$) identified in Fig. 3 $A$–$D$, respectively.
Simulated Anion Photoelectron Spectra

Figure 4A

Au_{15}^- (top 5)
Au$_{16}^-$ (top 5)

Figure 4B
Figure 4C

Au_{17}^- (top 6)
Figure 4D

Au$_{18}$- (top 6)
Fig. 4. Top-10 lowest-energy isomers of \( \text{Au}_{15} \) (A), \( \text{Au}_{16} \) (B), \( \text{Au}_{17} \) (C), \( \text{Au}_{18} \) (D), and \( \text{Au}_{19} \) (E) obtained from a basin-hopping global search combined with DFT optimization and total-energy calculation. The energy values (in eV) given beneath each isomer are the relative energy with respective to the leading lowest-energy isomer. The energy values in black are based on the PBE exchange-correlation functional (1), and the double numerical basis set with polarization functions, implemented in the DMOL\(^3\) package (2). Those isomers with their energy value within 0.2 eV from the leading lowest-energy isomer are all regarded as candidates for the lowest-energy structure to be compared with experimental data. Relative energies among these candidate lowest-energy isomers are further evaluated by using a modest and a large basis sets. The energy values in blue are based on optimization with the PBEPBE/LANL2DZ functional/basis set, implemented in the GAUSSIAN 03 package (3), and the energy values in red are based on single-point calculations at the PBEPBE/SDD+Au(2f)//PBEPBE/LANL2DZ level of theory, implemented in the GAUSSIAN 03 package (3). Here “SDD+Au(2f)” denotes the Stuttgart/Dresden ECP valence basis (4, 5) augmented by two sets of \( f \) polarization functions (exponents = 1.425, 0.468). The isomers enclosed by a black frame also are highlighted in Fig. 1B.

Notes

Au\textsubscript{15}\textsuperscript{−} (top10)

Figure 3A
Figure 3B

Au_{16}^- (top10)
Figure 3C

Au$_{17}^-$ (top10)
Figure 3D

$\text{Au}_{18}^{-} \text{ (top10)}$
Figure 3E
Table 2. The experimental adiabatic detachment energies (ADEs) for $\text{Au}_n^-$ ($n = 15$–$19$) measured from the threshold of the first photoelectron band

<table>
<thead>
<tr>
<th>Isomer</th>
<th>ADE, eV</th>
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<tbody>
<tr>
<td>$\text{Au}_{15}^-$</td>
<td>$3.61 \pm 0.03$</td>
</tr>
<tr>
<td>$\text{Au}_{16}^-$</td>
<td>$3.99 \pm 0.03$</td>
</tr>
<tr>
<td>$\text{Au}_{17}^-$</td>
<td>$4.03 \pm 0.03$</td>
</tr>
<tr>
<td>$\text{Au}_{18}^-$</td>
<td>$3.24 \pm 0.03$</td>
</tr>
<tr>
<td>$\text{Au}_{19}^-$</td>
<td>$3.71 \pm 0.03$</td>
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