SUPPORTING INFORMATION

On the Structure of the thiolated Au₁₃₀ Cluster

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Part I. **Figure S1.** UV/Vis spectrum of the Au₁₃₀ nanocluster recorded prior to spotting in MALDI-MS.

Figure S2. Comparison between calculated optical absorption spectra of Au₁₃₀(SH)₅₀ and Au₁₃₀[(SH)₂]₁₀[(SCH₂CH=CHCH₂S)₂]₁₅ clusters.

Part II. **Figure S3.** MALDI TOF generated mass spectra of Au₁₃₀. (Explain those 5 spectra with 29 KDa).

Part III. **Figure S4.** Relaxed model of the Au₁₃₀[(SH)₂]₁₀[(SCH₂CHCHCH₂S)₂]₁₅ cluster. This structure contains 130 gold and 80 sulfur atoms. Proposed model holds S-S bonds.

Figure S5. Raman spectra of Au₁₄₄(SR)₆₀ and Au₁₃₀(SR)_{50/80} clusters.

Part IV. **Figure S6.** Atlas of Simulated diffraction patterns obtained from the relaxed Au₁₃₀ model.

Part V. **Figure S7.** Map of Simulated images and diffraction patterns obtained from the relaxed Au₁₃₀ model.

Figure S8. Comparison between a) experimental, b) filtered image, and c) relaxed Au₁₃₀ model. H atoms are removed for simplicity.

Figure S9. Comparison of calculated XRD patterns of Au₁₃₀(SH)₅₀ and Au₁₃₀[(SH)₂]₁₀[(SCH₂CH=CHCH₂S)₂]₁₅ clusters.

Part VI.

Supplementary Video 1. Experimental NBD pattern.

Supplementary Video 2. Simulated electron diffraction pattern, direction <1-10>.

Supplementary Video 3. Simulated electron diffraction pattern, direction <010>.

Supplementary Video 4. Simulated electron diffraction pattern, direction <110>.

Supplementary Video 5. Simulated electron diffraction pattern, direction <100>.

Supplementary Video 6. Simulated electron diffraction pattern, direction <111>.

Supplementary Video 7. Simulated electron diffraction pattern, direction <112>.

Part VII. Cartesian coordinates of the Au₁₃₀(SH)₅₀ cluster.

Part I

Figure S1. UV/Vis spectrum of the Au₁₃₀ nanocluster recorded prior to spotting in MALDI-MS.

Figure S2. Comparison between calculated optical absorption spectra. Black curve refers to the Au₁₃₀(SH)₅₀ cluster and blue curve depicts the profile of the Au₁₃₀[(SH)₂]₁₀[(SCH₂CH=CHCH₂S)₂]₁₅ cluster. Dotted lines show the position of the peaks discussed in the manuscript.

Figure S3. MALDI TOF generated mass spectra of Au₁₃₀. (Explain those 5 spectra with 29 KDa).

Figure S4. Relaxed model of the $\text{Au}_{130}[(\text{SH})_2]_{10}[(\text{SCH}_2\text{CHCHCH}_2\text{S})_2]_{15}$ cluster. This structure contains 130 gold and 80 sulfur atoms. Proposed model holds S-S bonds.

Figure S5. Raman spectra of $\text{Au}_{144}(\text{SR})_{60}$ and $\text{Au}_{130}(\text{SR})_{50/80}$. It is important to mention that the Au_{144} spectrum is not smoothed while Au_{130} it does. The band at 519 cm^{-1} was attributed to the S-S bond. For the assignment of the band of S-S peak see reference below.

Szafranski, C. A.; Tanner, W.; Laibinis, P. E.; Garrel, R. L. Surface-Enhanced Raman Spectroscopy of Aromatic Thiols and Disulfides on Gold Electrodes. *Langmuir*, **1998**, 14, 3570-3579.

Part IV

Figure S6. Atlas of Simulated diffraction patterns obtained from the relaxed Au_{130} model.

Part V

Figure S7. Map of simulated images and diffraction patterns obtained from the relaxed Au_{130} model.

Figure S8. Comparison between a) experimental, b) filtered image and c) relaxed Au_{130} model. H atoms are removed for simplicity.

Figure S9. Comparison of calculated XRD patterns of $\text{Au}_{130}(\text{SH})_{50}$ and $\text{Au}_{130}[(\text{SH})_2]_{10}[(\text{SCH}_2\text{CH}=\text{CHCH}_2\text{S})_2]_{15}$ clusters. Both patterns are in agreement with Fig. 3 of the reference 18.

Part VII

Cartesian coordinates of the Au₁₃₀(SH)₅₀ cluster.

Au -0.11399517 -0.01834512 -6.11814486

Au -0.08456148 0.00442431 -2.90770160

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