SUPPORTING INFORMATION

New insight on the structure of thiolated gold clusters. A structural prediction of the \( \text{Au}_{187}(\text{SR})_{68} \) cluster

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Part I. Comparison of simulated XRD patterns of thiolated \( \text{Au}_{25} \), and \( \text{Au}_{38} \) clusters.

Part II. Bond distances of the optimized \( \text{Au}_{187}(\text{SH})_{68} \) model.
Figure S1. Comparison of the experimental (upper panel) and simulated curve of \( \text{Au}_{25}(\text{SR})_{18} \) cluster. Red curve represents the smoothed one of the experimental XRD pattern. Theoretical curve corresponds with the structure reported in ref. 19.
Figure S2. Comparison of the experimental (upper panel) and simulated curve of Au$_{38}$(SR)$_{24}$ cluster. Red curve represents the smoothed one of the experimental XRD pattern. Theoretical curve corresponds with the structure reported in ref. 20.
Figure S3. Bond length of relaxed Au$_{187}$(SH)$_{68}$ cluster.