SUPPORTING INFORMATION

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

Alfredo Tlahuice-Flores

CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450, México

Email: tlahuicef@gmail.com

Part I. Comparison of simulated XRD patterns of thiolated Au_{25}, and Au_{38} clusters.

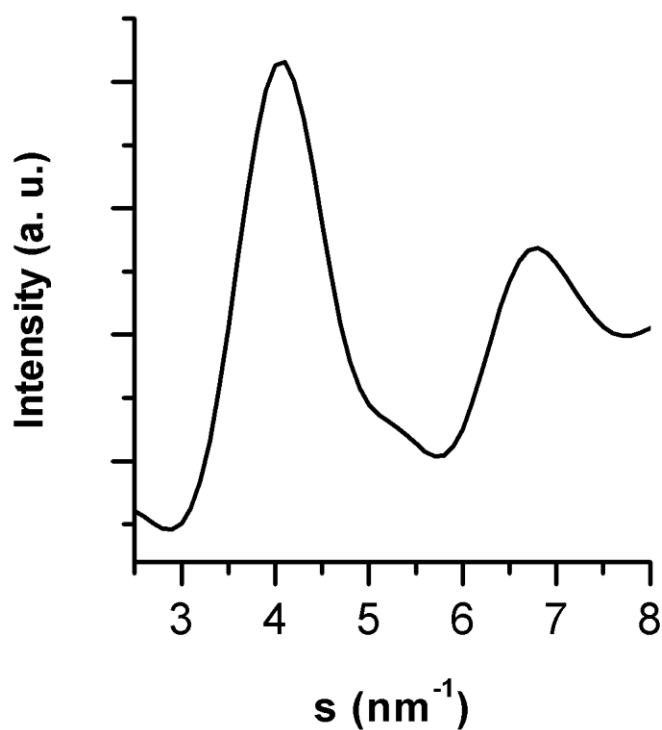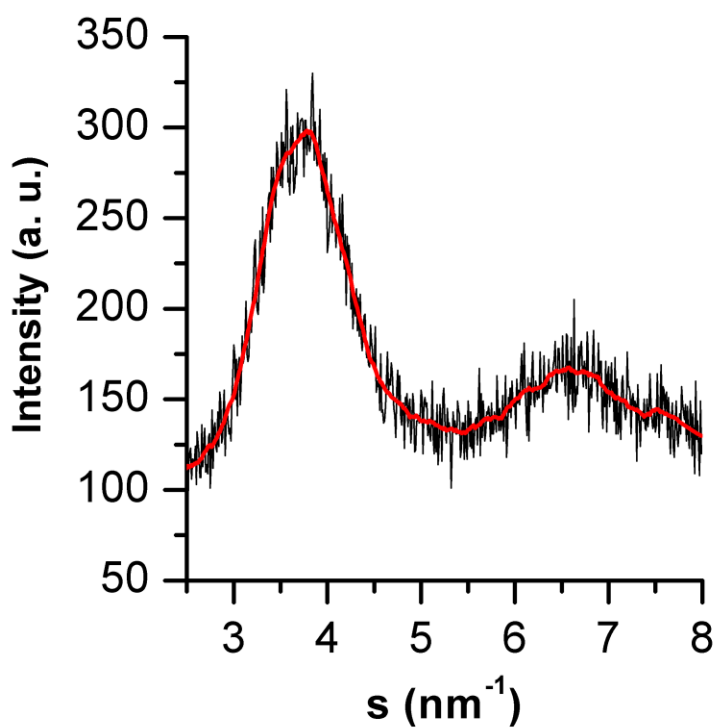Part II. Bond distances of the optimized $Au_{187}(SH)_{68}$ model.

Figure S1. Comparison of the experimental (upper panel) and simulated curve of $Au_{25}(SR)_{18}$ cluster. Red curve represents the smoothed one of the experimental XRD pattern. Theoretical curve corresponds with the structure reported in ref. 19.
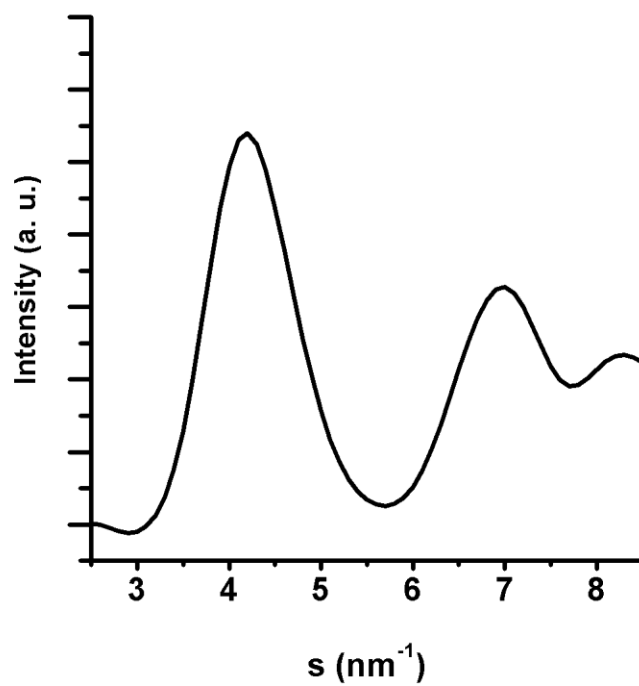
Figure S2. Comparison of the experimental (upper panel) and simulated curve of $Au_{38}(SR)_{24}$ cluster. Red curve represents the smoothed one of the experimental XRD pattern. Theoretical curve corresponds with the structure reported in ref. 20
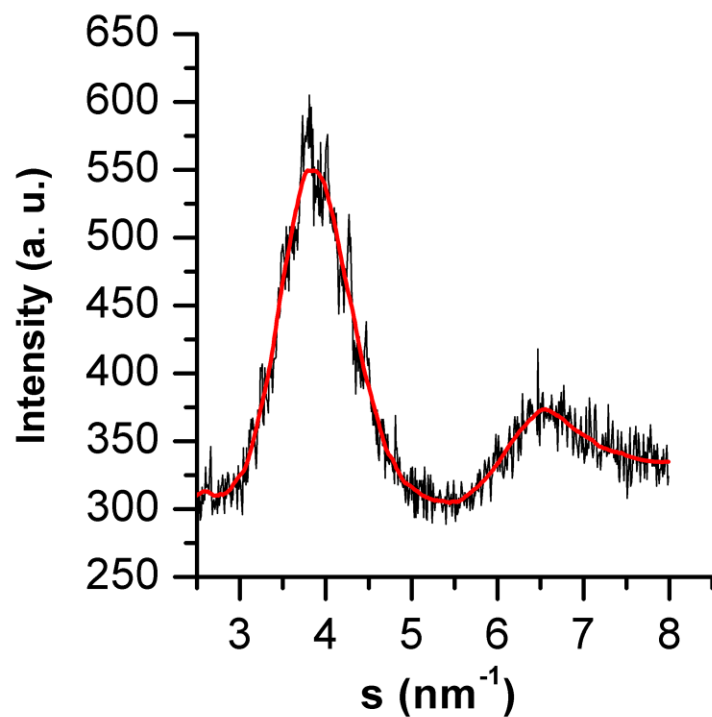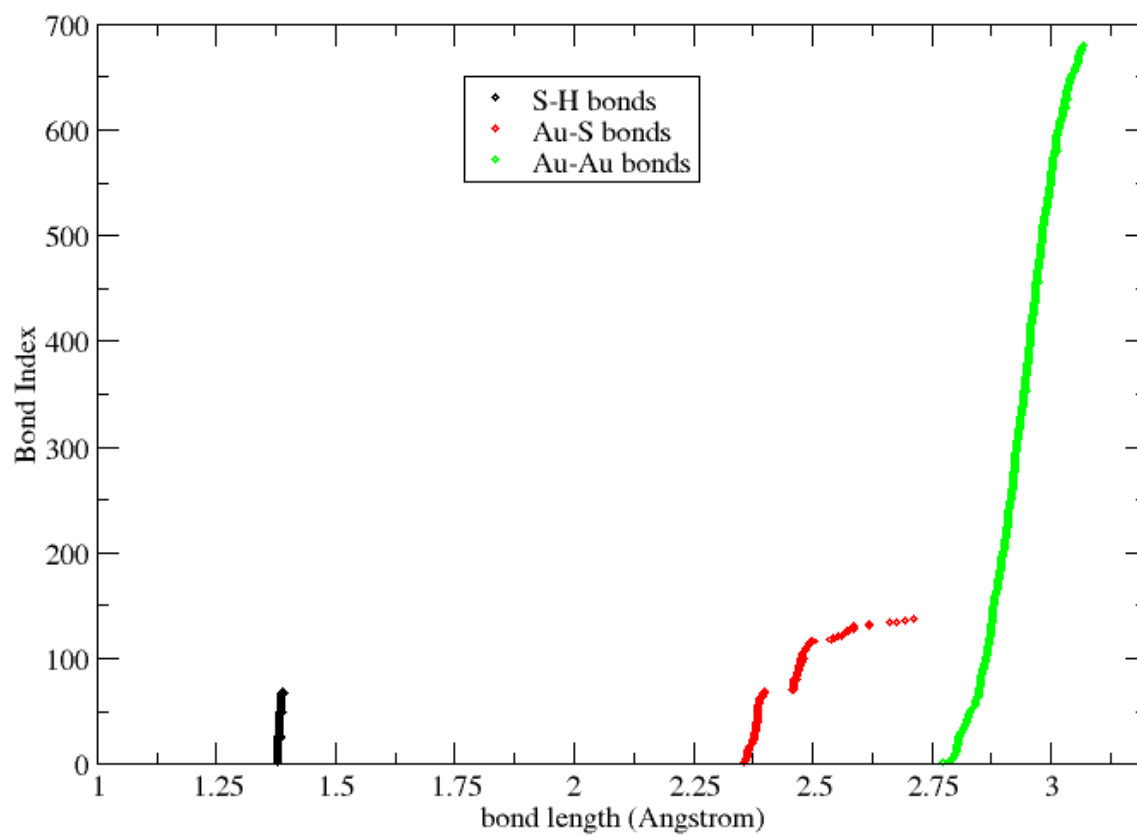
PART II

Figure S3. Bond length of relaxed $Au_{187}(SH)_{68}$ cluster.