SUPPORTING INFORMATION

for

Ligand-Core NLO-phores: a combined experimental and theoretical approach of the two-photon absorption and two-photon excited emission properties of small ligated silver nanoclusters

Isabelle Russier-Antoine, Franck Bertorelle, Nathalie Calin, Željka Sanader, Marjan Krstić, Clothilde Comby-Zerbino, Philippe Dugourd, Pierre-François Brevet, Vlasta Bonačić-Koutecký,* and Rodolphe Antoine*

Electronic Supplementary Material (ESI) for Nanoscale

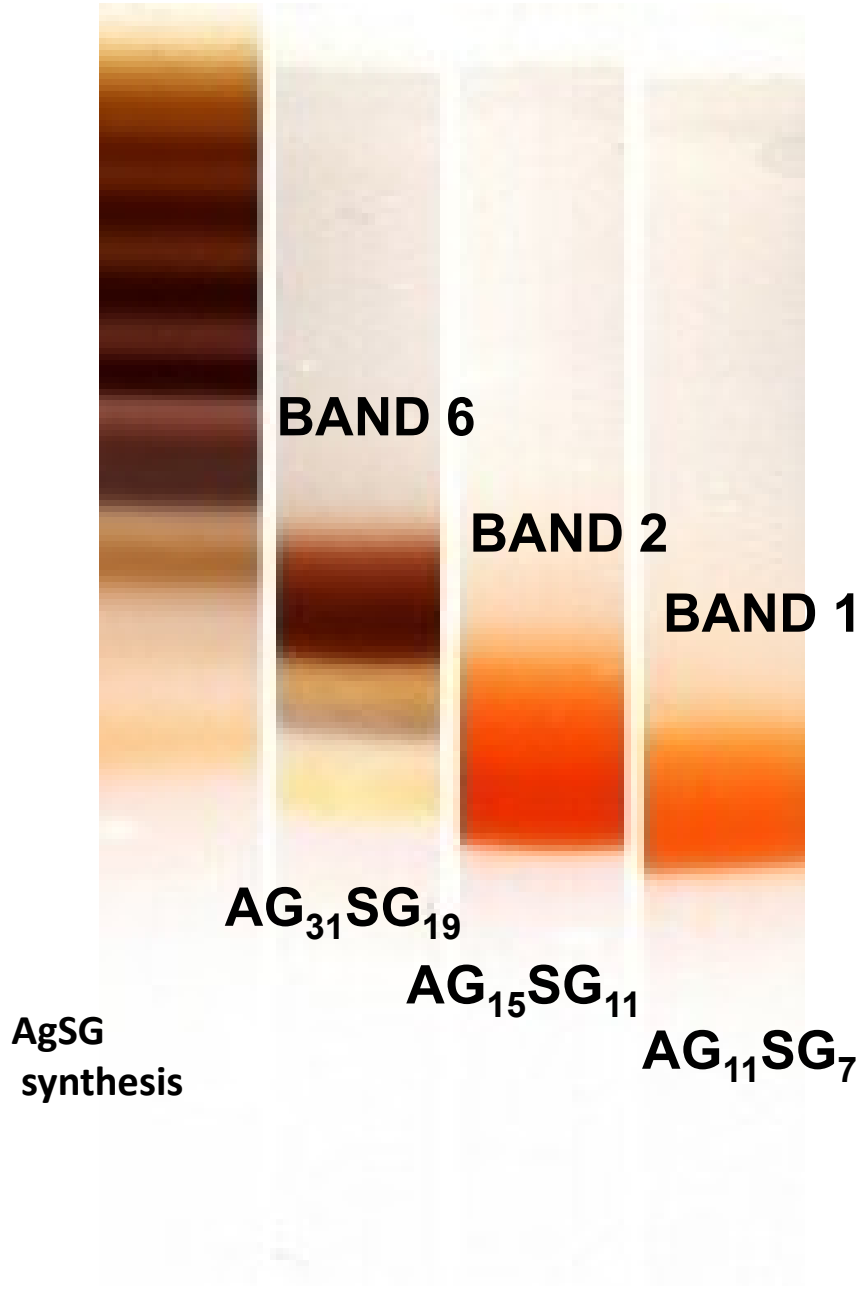

Figure S1 : : PAGE for Ag:SG clusters using (left) Bigioni synthesis (Santosh Kumar, Michael D. Bolan, and Terry P. Bigioni. Journal of the American Chemical Society 2010 132 (38), 13141-13143) and (right) our “size-focusing” synthesis.

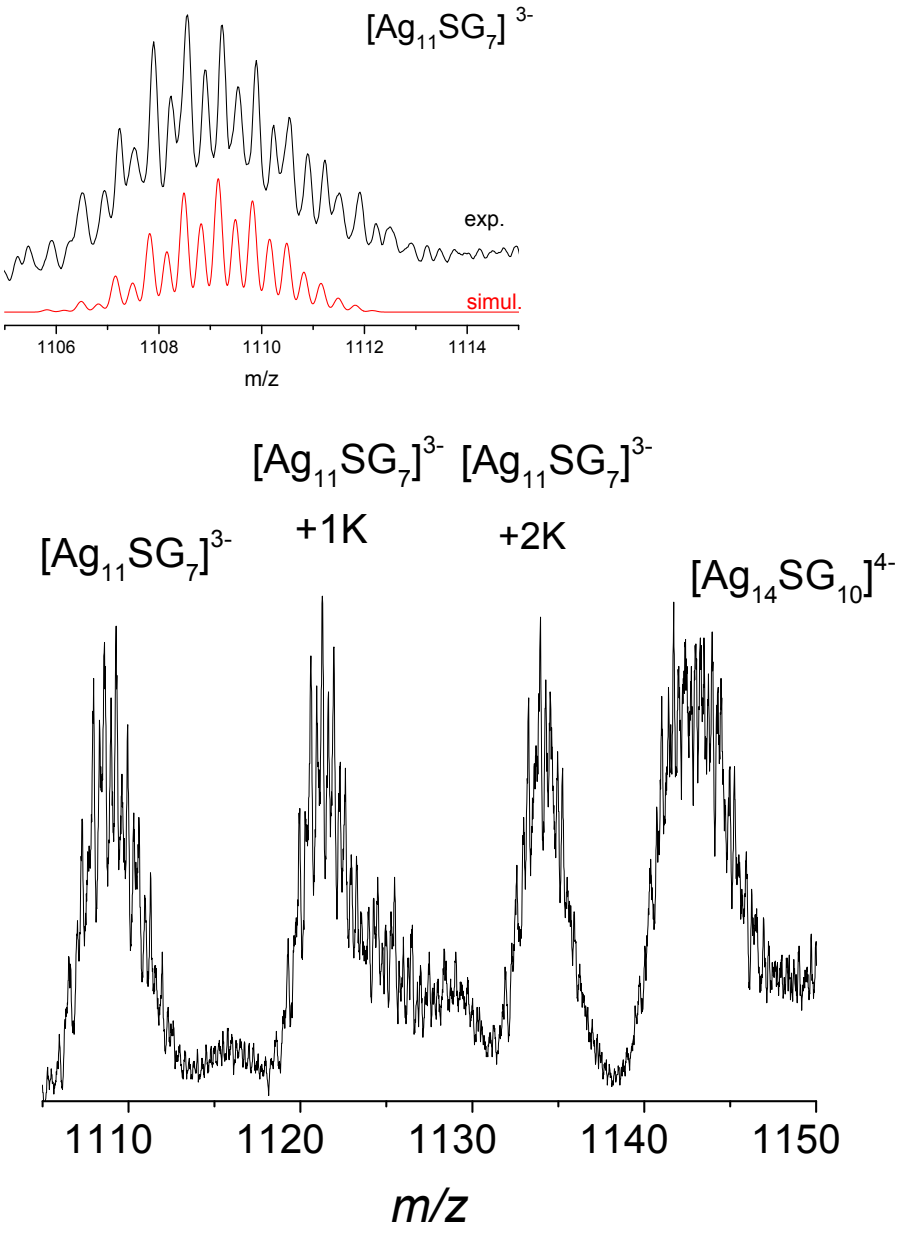

Figure S2 : (bottom) ESI MS of the clusters in the negative ion mode showing −2 and −3 charged species along with some other thiolates. (top) Experimental spectrum (black trace) is in good agreement with the calculated mass spectrum (red trace) of the Ag11SG7 species. Note that multiple potassium attachments to glutathione ligand are observed in mass spectra.

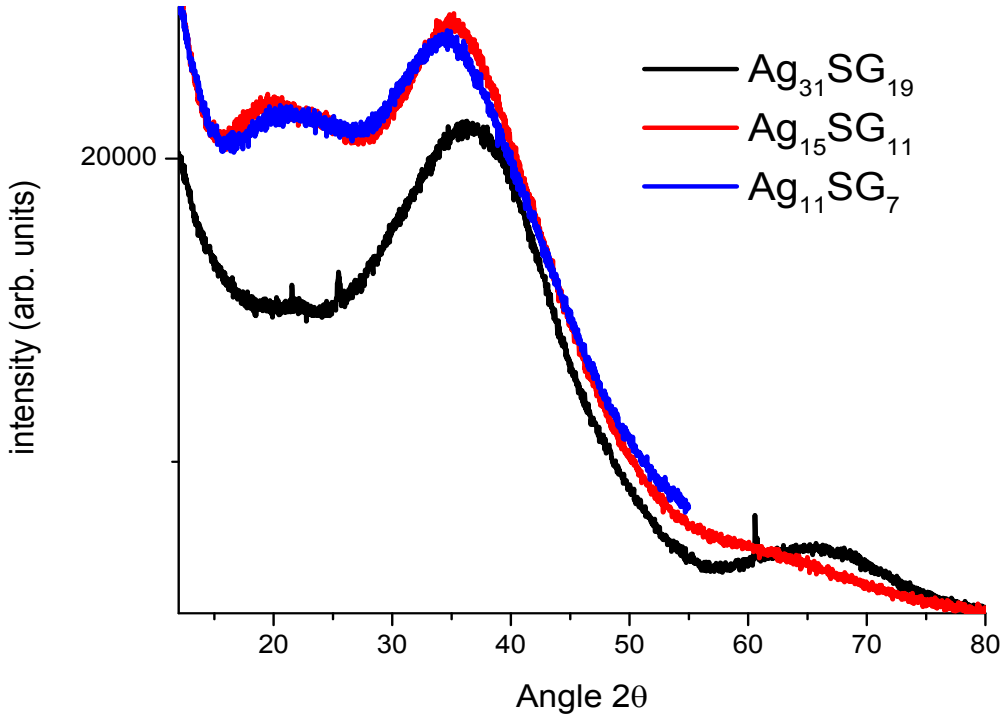

Figure S3 : XRD patterns of Ag(SG) nanoclusters.

Average core diameter (from DFT structures)		EXP
AG11L7	0.54 nm	0.49 nm
AG15L11	0.50 nm	0.49 nm
Ag31L19	0.67 nm	0.6 nm

TABLE S1 : Experimental (from XRPD patterns) and calculated (from DFT structures) core diameters for Ag(SG) nanoclusters.

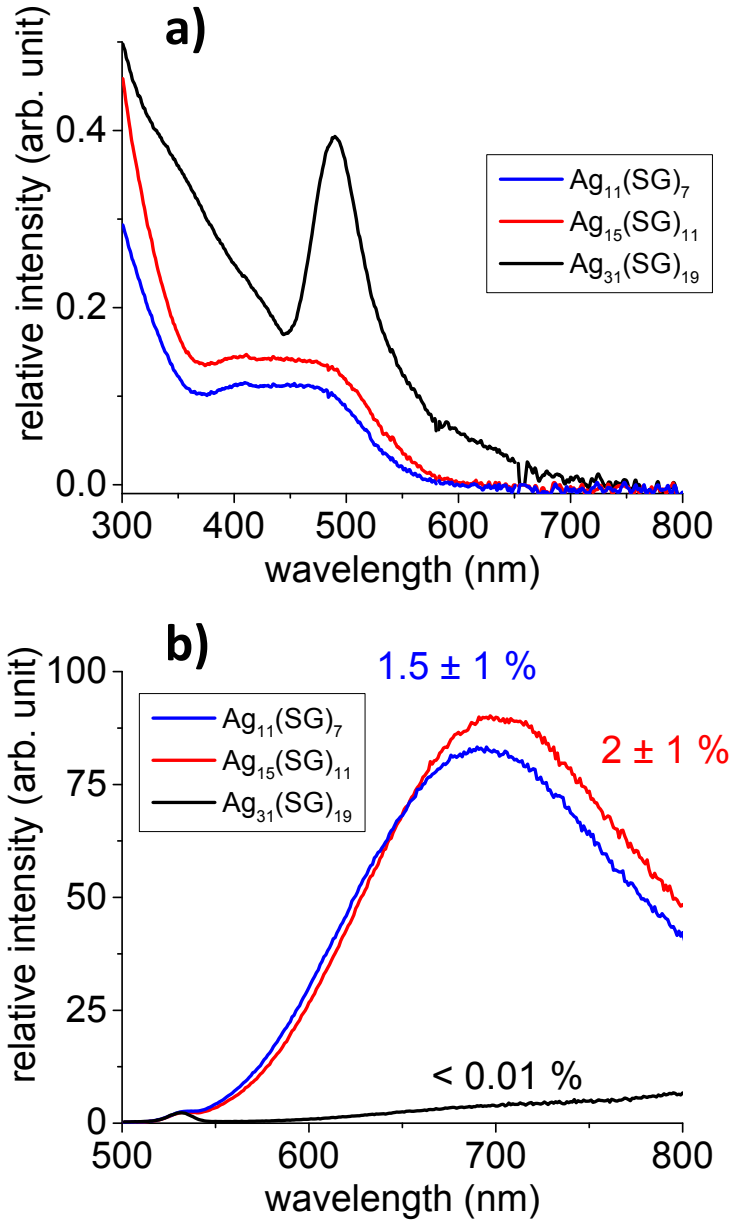

Figure S4 : Optical absorption (a) and fluorescence (b) spectra (with an excitation at 450 nm) for the three cluster sizes (Ag11(SG)7, Ag15(SG)11 and Ag31(SG)19).

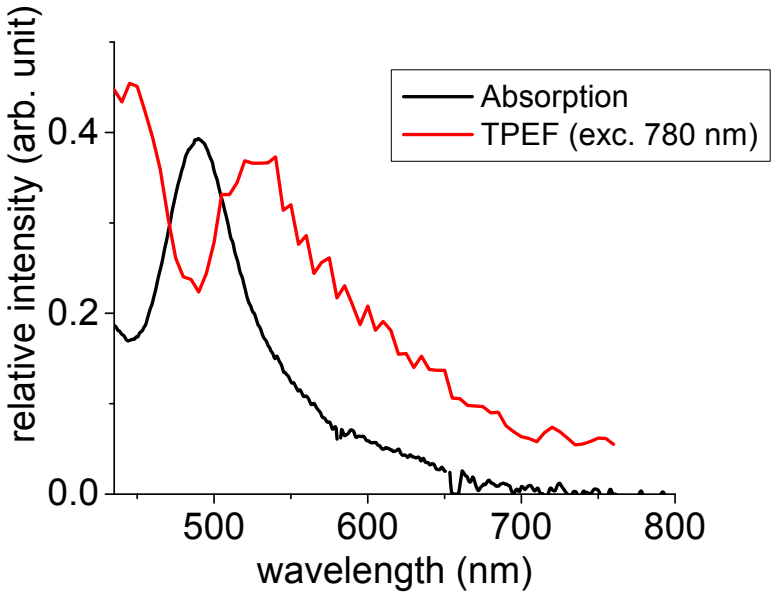

Figure S5 : TPEF spectrum (red) reported for band 6 ($Ag_{31}(SG)_{19}$) with its absorption spectrum (black).

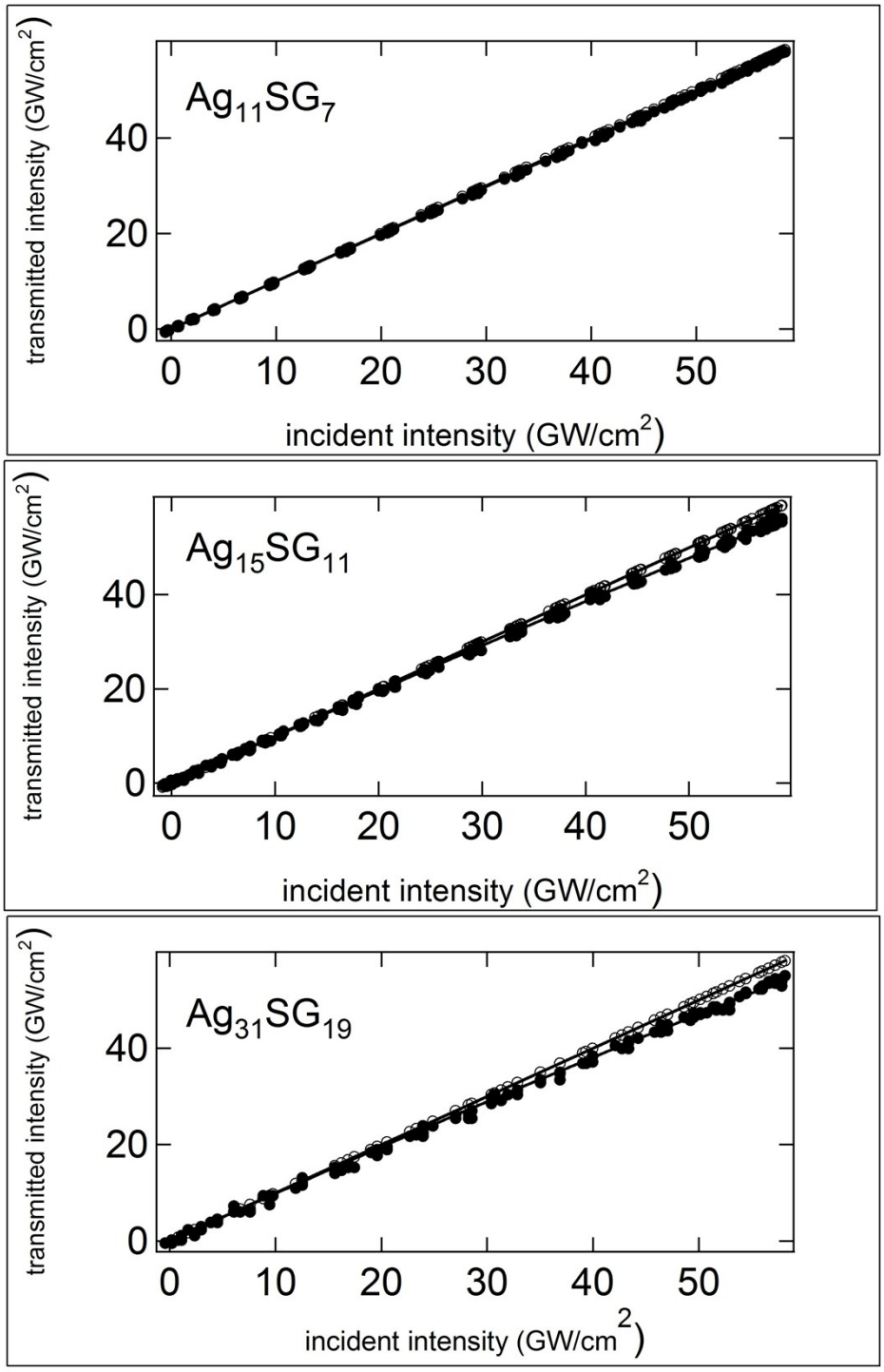

Figure S6 : Transmitted intensity recorded at 800 nm (empty circles) with a cell of water, (filled circles) with the nanoclusters solution. Solid lines are fit using a nonlinear absorption.

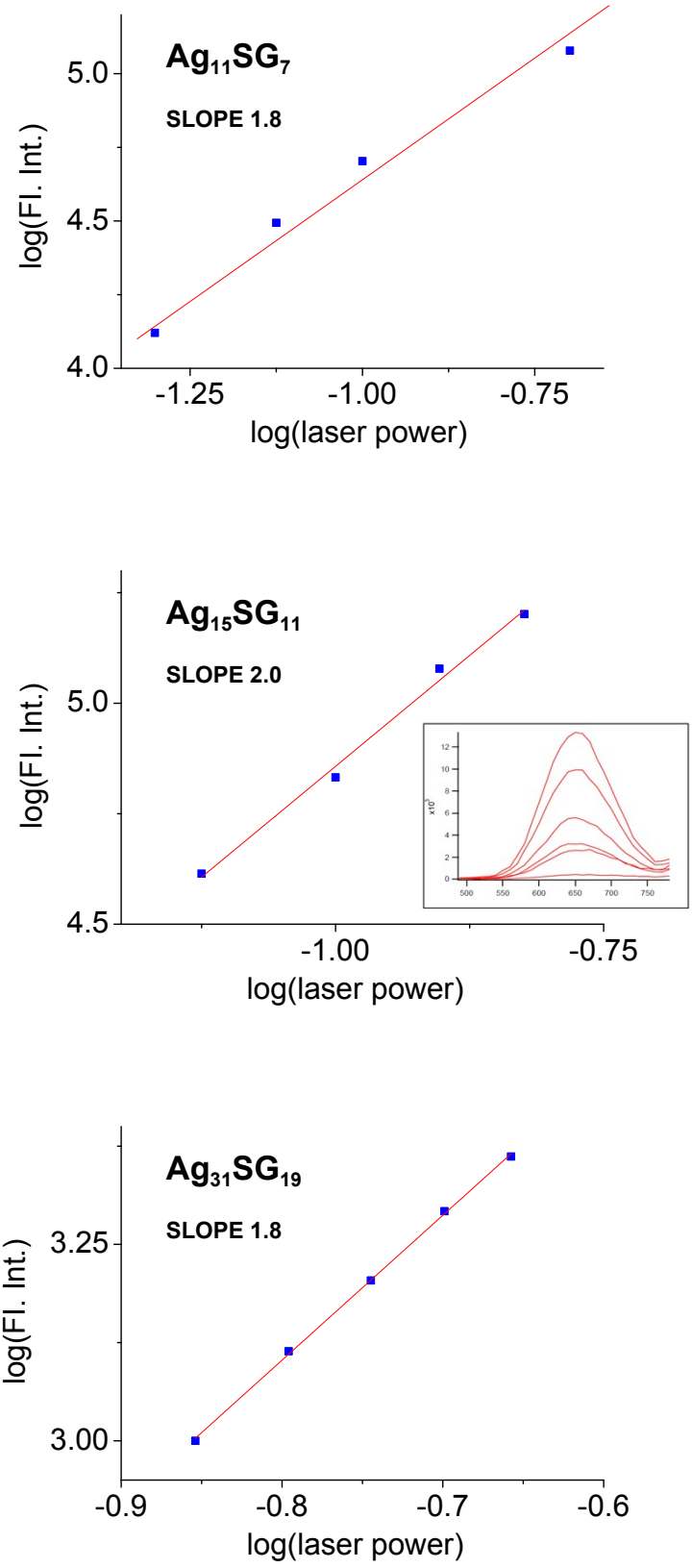

Figure S7 : Power dependence of emission at different pump powers for Ag(SG) clusters after excitation at 800 nm. Two-photon emission spectra of $Ag_{15}(SG)_{11}$ for different pump powers are also provided (inset of central panel).