Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Effect of the Charge State on the structure of the Au_{60} cluster

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Figure S1. Octahedra distribution.

Figure S2. Au_{60} cluster with a 2+ charge state. Polyhedral approach analysis.

Figure S3. Tetrahedra distribution with respect to octahedral blocks.

Figure S4. Compact region and the polyhedral blocks.

Figure S5. Two more perfect octahedra and their distribution along the Au_{60} cluster with a 2+ charge state.

Figure S6. Distribution of the 12 more compact tetrahedra in the Au_{60} cluster holding a 2+ charge state.

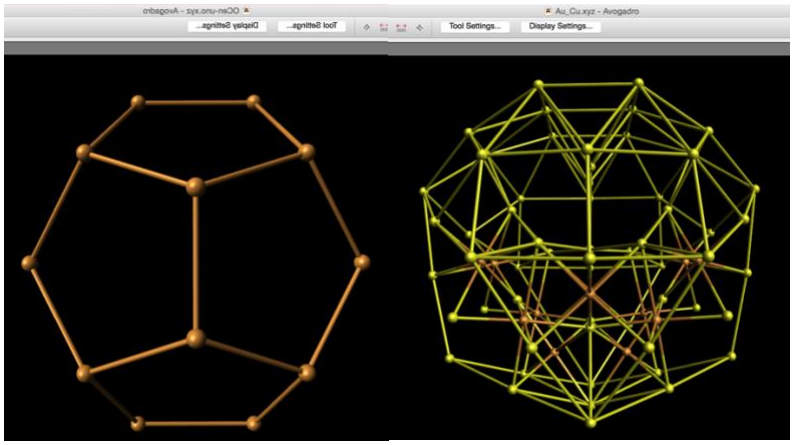
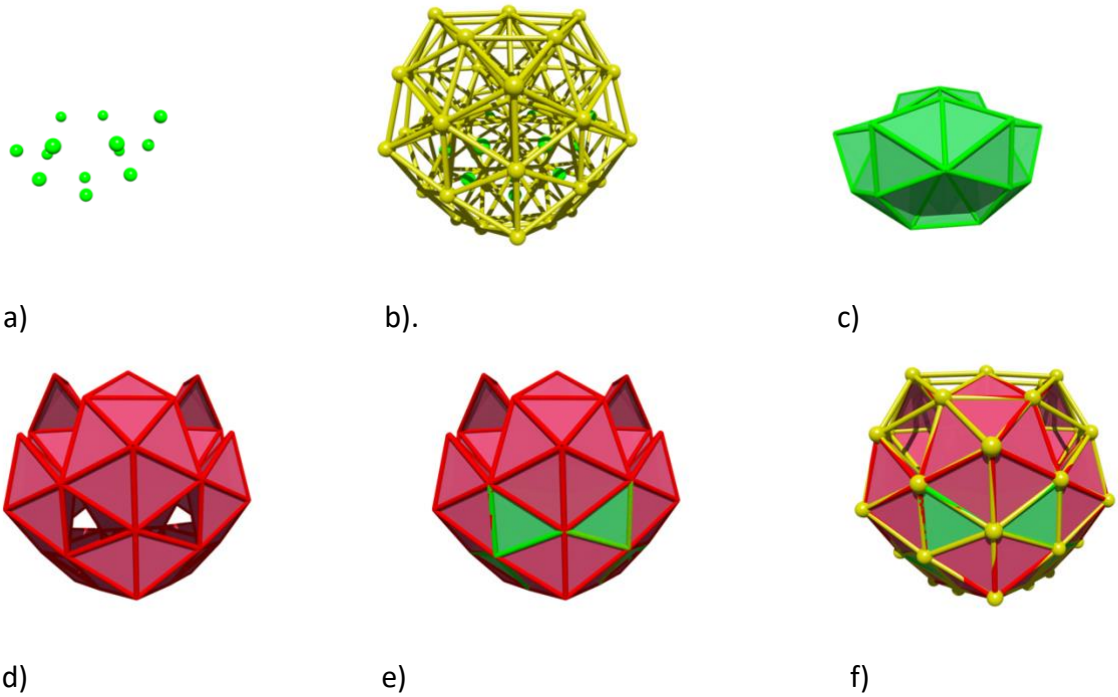


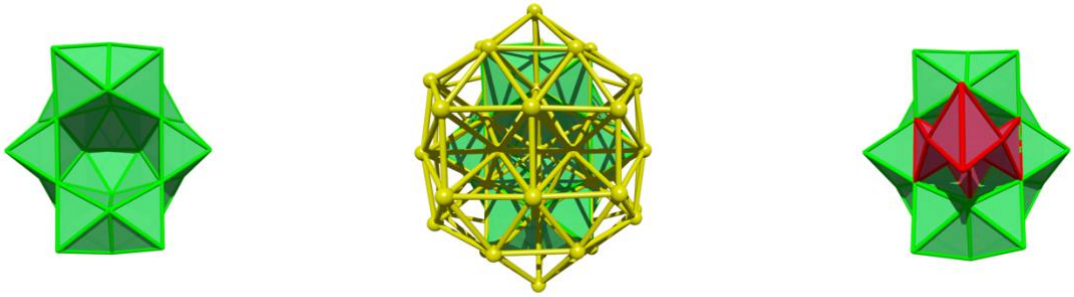
Figure S1. Centre of 12 octahedra forming an arrangement of four pentagonal rings fused as in the dodecahedron. To the right is depicted the distribution of the octahedral blocks in the total structure of the 2+ Au_{60} cluster.



a) b). c)

d) e) f)

Figure S2. Hidden view of the 2+ Au_{60} cluster related to the Figure 1. a) Center of the 12 octahedral blocks, b) Distribution of the octahedra in the cluster, c) Octahedra showing triangular faces, d) Tetrahedra distribution, d) Both type of polyhedral blocks, and f) full view of the structure.



a) b). c)

Figure S3. a) The octahedra distribution in the 2+ Au_{60} cluster is forming a compact region. b) This distribution is shown and c) 4 tetrahedra are constituting the inner Au_{13} core, attesting the major induced distortion.

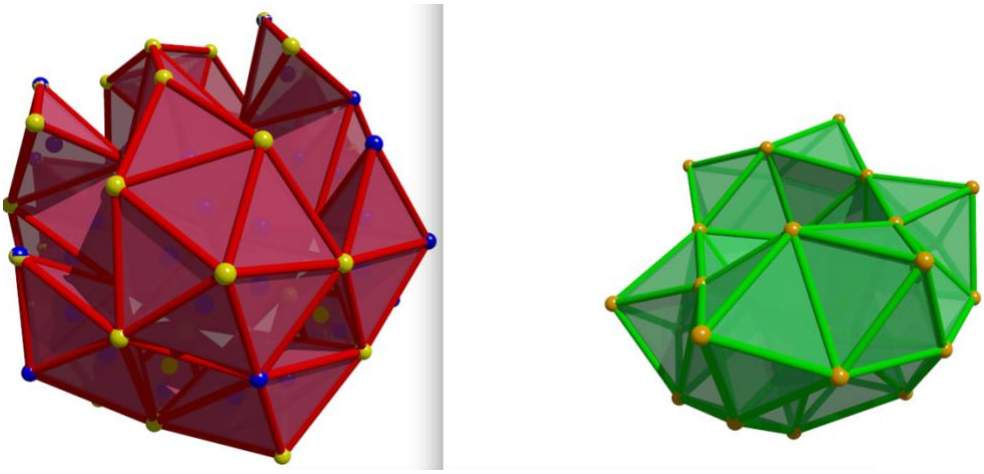


Figure S4. The octahedra distribution in the 2+ Au_{60} cluster. Interestingly, the octahedra are located in the more compact region. The orientation of the structure is the same for both polyhedral blocks.

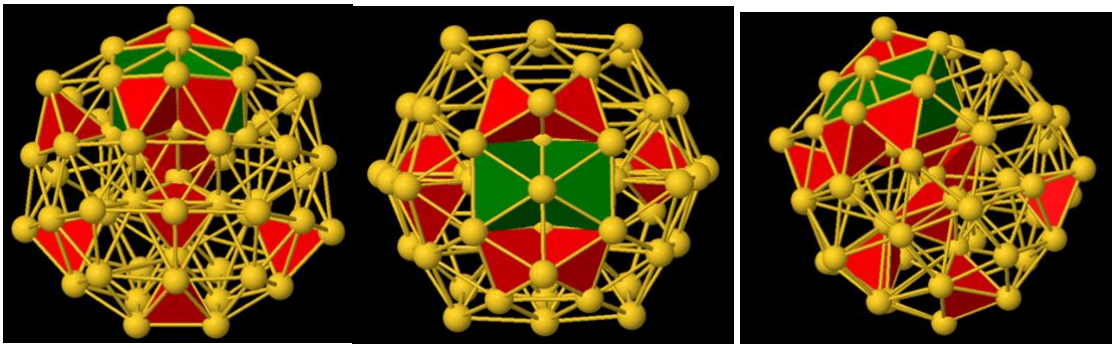


Figure S5. Distribution of the two more compact/perfect octahedra (in green color) along the structure of the 2+ Au_{60} cluster. It is evident the presence of a symmetry plane and tetrahedra (in red color) also are distributed following this symmetric pattern.

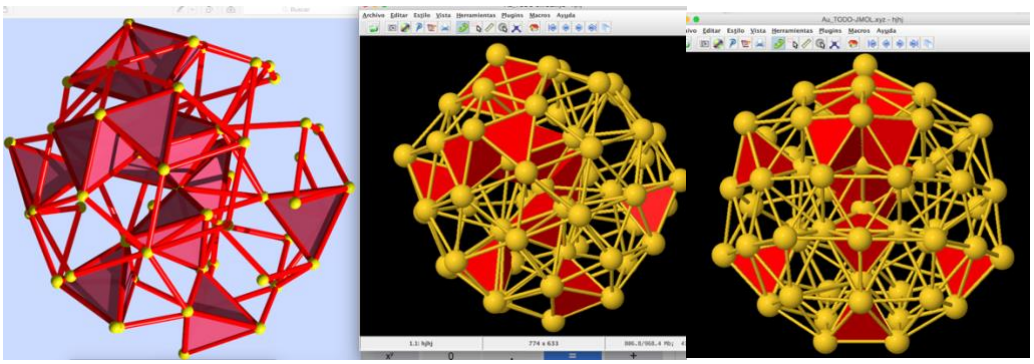


Figure S6. 12 more compact tetrahedra distributed along the whole structure of the 2+ Au_{60} cluster. Only four tetrahedra are forming the inner Au13 core, the rest are dispersed over all the structure.