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


## Supplementary information

# The lowest-energy structure of the gold cluster $Au_{10}$: Planar *vs.* nonplanar?

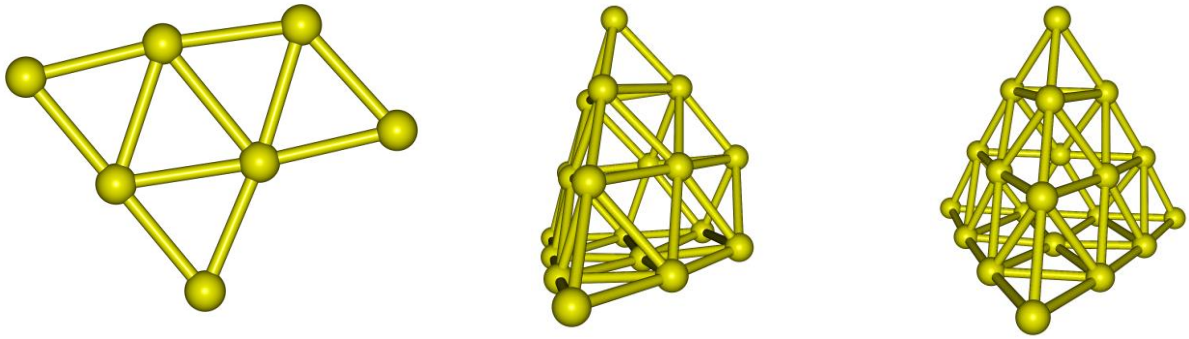
**Pham Vu Nhat,[1,*] Nguyen Thanh Si,[1] Nguyen Thi Nhat Hang,[2] Minh Tho Nguyen[3,*]**

[1] *Department of Chemistry, Can Tho University, Can Tho, Viet Nam.*

[1] *Faculty of Food Science and Technology, Thu Dau Mot University, Thu Dau Mot, Vietnam*

[3] *Institute for Computational Science and Technology (ICST), Quang Trung Software City, Ho Chi Minh City, Vietnam.*

Emails: nhat@ctu.edu.vn; tho.nm@icst.org.vn; minh.nguyen@kuleuven.be



$Au_7$ $Au_{19}$ $Au_{20}$

**Figure S1**. The most stable forms of $Au_7$, $Au_{19}$ and $Au_{20}$ clusters

**Table S1.** Optimized geometries and Cartesian coordinates of some lower-lying isomers of the neutral $Au_{10}$ cluster (PBE/cc-pVTZ-PP, angstrom).

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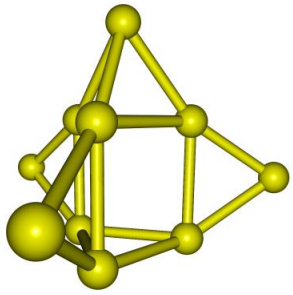
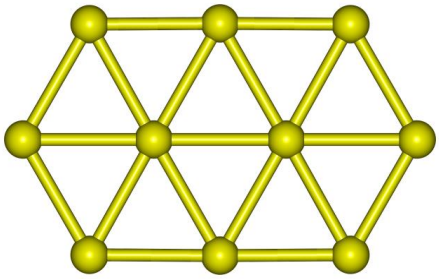
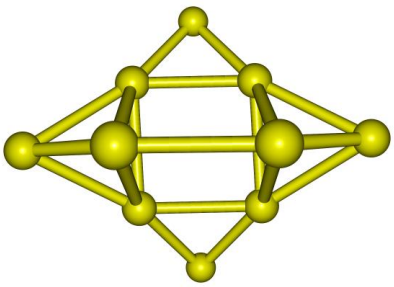
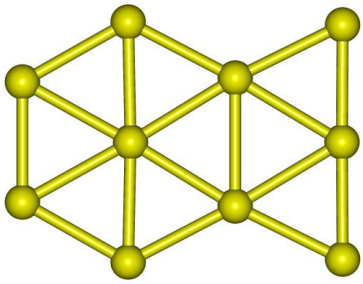
| Geometry | Cartesian coordinates | | | |
|---|---|---|---|---|
|  **Iso_1**, $C_{3v}$ (0.0) | 79 | 0.000000000 | 1.536819501 | -1.700673252 |
| | 79 | -1.330924726 | -0.768409746 | -1.700673252 |
| | 79 | -1.398818771 | -0.807608388 | 1.018978694 |
| | 79 | 0.000000000 | 1.615216786 | 1.018978694 |
| | 79 | -3.311973428 | -1.912168748 | -0.367824917 |
| | 79 | 0.000000000 | 3.824337495 | -0.367824917 |
| | 79 | 1.398818771 | -0.807608388 | 1.018978694 |
| | 79 | 1.330924726 | -0.768409746 | -1.700673252 |
| | 79 | 0.000000000 | 0.000000000 | 3.148554226 |
| | 79 | 3.311973428 | -1.912168748 | -0.367824917 |
|  **Iso_2**, $D_{2h}$ (0.1) | 79 | 0.000000000 | 2.378678171 | 0.000000000 |
| | 79 | 0.000000000 | -2.378678171 | 0.000000000 |
| | 79 | 0.000000000 | -2.361519170 | 2.688941193 |
| | 79 | 0.000000000 | 0.000000000 | 4.054456292 |
| | 79 | 0.000000000 | 2.361519170 | 2.688941193 |
| | 79 | 0.000000000 | 0.000000000 | 1.363967098 |
| | 79 | 0.000000000 | 0.000000000 | -1.363967098 |
| | 79 | 0.000000000 | 2.361519170 | -2.688941193 |
| | 79 | 0.000000000 | -2.361519170 | -2.688941193 |
| | 79 | 0.000000000 | 0.000000000 | -4.054456292 |
|  **Iso_3**, $C_{2v}$ (1.6) | 79 | -1.978019142 | -0.074734005 | -0.361666026 |
| | 79 | -0.881880064 | -0.965042070 | 2.034759146 |
| | 79 | 0.881880064 | 0.965042070 | 2.034759146 |
| | 79 | -0.124628009 | 1.961610141 | -0.356060026 |
| | 79 | -2.387779172 | 2.162713156 | -1.687862121 |
| | 79 | 1.978019142 | 0.074734005 | -0.361666026 |
| | 79 | 0.124628009 | -1.961610141 | -0.356060026 |
| | 79 | -2.387779172 | -2.640260190 | 0.370829027 |
| | 79 | 2.387779172 | 2.640260190 | 0.370829027 |
| | 79 | 2.387779172 | -2.162713156 | -1.687862121 |
|  **Iso_4**, $C_{2v}$ (3.3) | 79 | 0.000000000 | 2.677978193 | -1.440667104 |
| | 79 | 0.000000000 | -2.677978193 | -1.440667104 |
| | 79 | 0.000000000 | -1.339678096 | -3.784619272 |
| | 79 | 0.000000000 | 1.339678096 | -3.784619272 |
| | 79 | 0.000000000 | 1.439073103 | 0.937432067 |
| | 79 | 0.000000000 | 0.000000000 | -1.378696099 |
| | 79 | 0.000000000 | -1.439073103 | 0.937432067 |
| | 79 | 0.000000000 | -2.609616188 | 3.323428239 |
| | 79 | 0.000000000 | 0.000000000 | 3.307547238 |
| | 79 | 0.000000000 | 2.609616188 | 3.323428239 |

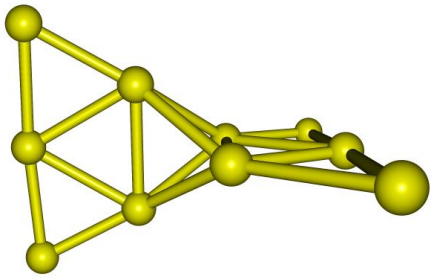
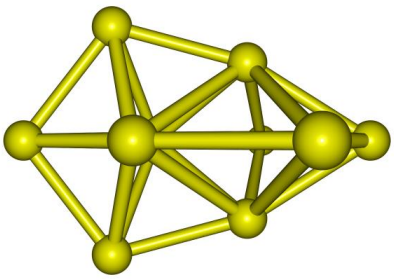
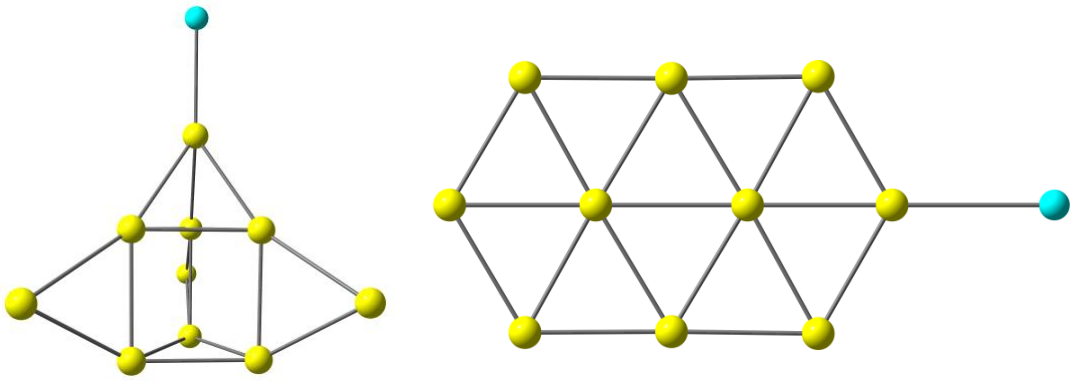
| | | | | |
|---|---|---|---|---|
|  **Iso_5**, $D_{2d}$ (5.9) | 79 | 0.000000000 | 2.627777189 | 3.317739239 |
| | 79 | 0.000000000 | 1.372276099 | 0.985725071 |
| | 79 | 0.000000000 | 0.000000000 | 3.444709248 |
| | 79 | -1.372296099 | 0.000000000 | -0.985730071 |
| | 79 | 0.000000000 | -2.627777189 | 3.317739239 |
| | 79 | 0.000000000 | -1.372276099 | 0.985725071 |
| | 79 | 1.372296099 | 0.000000000 | -0.985730071 |
| | 79 | -2.627780189 | 0.000000000 | -3.317758239 |
| | 79 | 2.627780189 | 0.000000000 | -3.317758239 |
| | 79 | 0.000000000 | 0.000000000 | -3.444658248 |
|  **Iso_6**, $D_{2d}$ (6.7) | 79 | 0.000000000 | 0.000000000 | 3.377222243 |
| | 79 | -2.203883159 | 0.000000000 | 1.649601119 |
| | 79 | -1.538398111 | 0.000000000 | -0.973807070 |
| | 79 | 0.000000000 | 1.538398111 | 0.973807070 |
| | 79 | 0.000000000 | -1.538398111 | 0.973807070 |
| | 79 | 1.538398111 | 0.000000000 | -0.973807070 |
| | 79 | 2.203883159 | 0.000000000 | 1.649601119 |
| | 79 | 0.000000000 | -2.203883159 | -1.649601119 |
| | 79 | 0.000000000 | 2.203883159 | -1.649601119 |
| | 79 | 0.000000000 | 0.000000000 | -3.377222243 |

**Table S2**. Free energies ΔG (kcal.mol$^{-1}$) of $Au_{10}$ isomers at different temperatures T = 100, 200 and 300 K

| **Method** | **LC-BLYP** | **PNO-LCCSD(T)-F12** | |
|---|---|---|---|
| Basis set | VTZ-PP | VTZ-PP | aVTZ-PP |
| | | **T = 100 K** | |
| **Iso_1** | 0.0 | 0.0 | 0.0 |
| **Iso_2** | 4.1 | 0.6 | 0.1 |
| **Iso_3** | 4.4 | 2 | 1.8 |
| **Iso_4** | 3.3 | 3.9 | 2.9 |
| **Iso_5** | 2.9 | 5.9 | 5.5 |
| **Iso_6** | 22.7 | 7.4 | 7.2 |
| | | **T = 200 K** | |
| **Iso_1** | 0.0 | 0.0 | 0.0 |
| **Iso_2** | 4.1 | 0.6 | 0.0 |
| **Iso_3** | 4.2 | 1.9 | 1.6 |
| **Iso_4** | 2.9 | 3.5 | 2.5 |
| **Iso_5** | 2.5 | 5.4 | 5.1 |
| **Iso_6** | 23.2 | 8.0 | 7.7 |
| | | **T = 300 K** | |
| **Iso_1** | 0.0 | 0.0 | 0.0 |
| **Iso_2** | 4.1 | 0.6 | 0.0 |
| **Iso_3** | 4.1 | 1.7 | 1.5 |
| **Iso_4** | 2.5 | 3.1 | 2.1 |
| **Iso_5** | 2.0 | 5.0 | 4.7 |
| **Iso_6** | 23.7 | 8.5 | 8.2 |

**Table S3.** Relative energies (kcal.mol$^{-1}$) of six lower-lying structures of $Au_{10}$ computed at different levels.

| | CCSD(T) | | | PNO-LCCSD(T)-F12 | | | |
|---|---|---|---|---|---|---|---|
| **Isomer** | VDZ-PP | aVDZ-PP | VTZ-PP | VDZ-PP | aVDZ-PP | VTZ-PP | aVTZ-PP |
| **Iso_1** | **0.0** | 1.2 | 2.0 | 2.0 | 0.8 | **0.0** | **0.0** |
| **Iso_2** | 2.8 | **0.0** | **0.0** | 1.5 | **0.0** | 0.6 | 0.1 |
| **Iso_3** | 0.4 | 2.3 | 3.8 | 1.6 | 2.7 | 1.6 | 1.8 |
| **Iso_4** | 3.2 | 3.2 | 3.2 | 5.8 | 3.5 | 4.3 | 3.3 |
| **Iso_5** | 6.7 | 5.4 | 6.7 | 8.2 | 6.0 | 6.3 | 5.9 |
| **Iso_6** | 1.5 | 6.9 | 10.0 | **0.0** | 7.0 | 7.0 | 6.7 |



Iso_1·Kr, 0.0 Iso_2·Kr, 6.0

**Fig. S1**. Optimized geometries and relative energy (kcal.mol$^{-1}$) of Iso_1·Kr and Iso_2·Kr complexes (LC-BLYP/cc-pVTZ-PP/cc-VTZ).

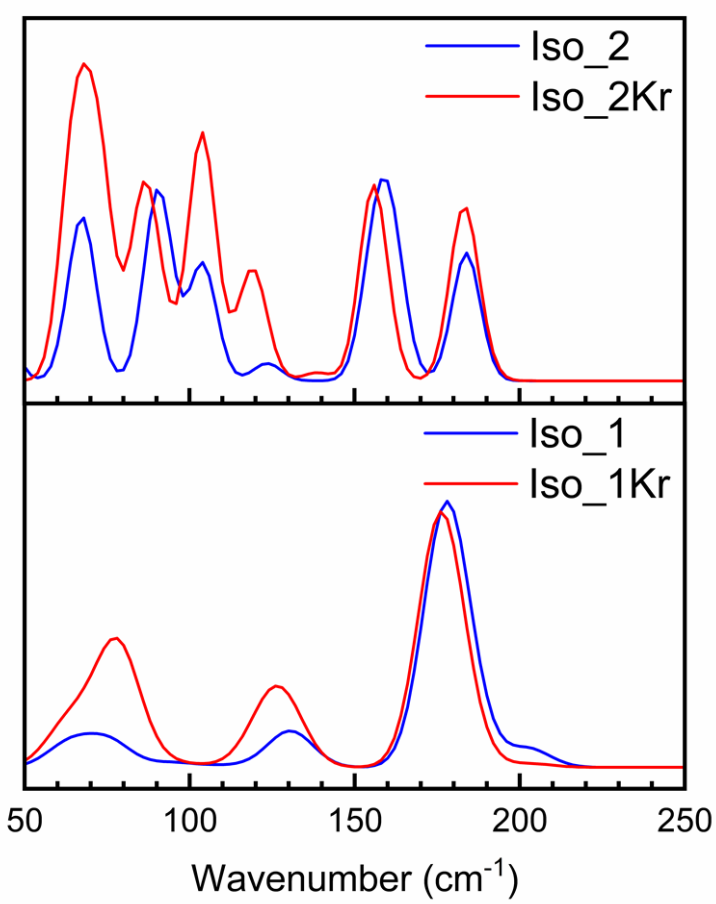



**Fig. S2**. Theoretical IR spectra of **Iso_1** and **Iso_2** isomers, and their complexes with the Kr atom.