

Supporting Information: Reply to ‘Comment on “Structural characterization, reactivity, and vibrational properties of silver clusters: A new global minimum for Ag₁₆”’ by P. V. Nhat, N. T. Si, L. V. Duong and M. T. Nguyen, Phys. Chem. Chem. Phys., 2021, 23, DOI: D1CP00646K

Peter L. Rodríguez-Kessler,^{*a} Adán R. Rodríguez-Domínguez,^b Desmond MacLeod-Carey,^{*a}
and Alvaro Muñoz-Castro^{*a}

^a Grupo de Química Inorgánica y Materiales Moleculares, Facultad de Ingeniería, Universidad Autónoma de Chile, El Llano Subercaseaux 2810, Santiago, Chile. E-mail: rodriguezkessler.p@gmail.com, desmond.macleod@uautonoma.cl, alvaro.munoz@uautonoma.cl

^b Instituto de Física, Universidad Autónoma de San Luis Potosí, San Luis Potosí 78000, México

1 Cartesian coordinates

1.1 The lowest energy structures of Ag₁₅ clusters calculated by using the Gaussian 09 program within the PW91/cc-pVDZ-PP approach.

15-1 geometry:

Ag	1.351848000	3.120689000	0.408251000
Ag	-1.114309000	-1.055441000	-2.056970000
Ag	0.191211000	1.258125000	-1.274935000
Ag	1.524352000	-1.175669000	-1.167923000
Ag	3.860983000	-1.064023000	0.411598000
Ag	1.660777000	0.403666000	1.344950000
Ag	-0.706917000	-0.989192000	0.854417000
Ag	1.638841000	-2.528763000	1.218002000
Ag	-0.848665000	1.678195000	1.453276000
Ag	-0.501996000	-3.351984000	-0.477939000
Ag	-3.062318000	-1.941693000	-0.283989000
Ag	3.006819000	1.253100000	-0.946636000
Ag	-2.558738000	0.928874000	-0.718499000
Ag	-3.110757000	-0.030943000	1.830357000
Ag	-1.331131000	3.495057000	-0.593959000

15-2 geometry:

Ag	-1.435826000	1.390222000	-0.338505000
Ag	0.000000000	2.048856000	2.087122000
Ag	1.905994000	0.000000000	2.015020000
Ag	1.435826000	-1.390222000	-0.338505000
Ag	1.435826000	1.390222000	-0.338505000
Ag	-1.905994000	0.000000000	2.015020000
Ag	-1.435826000	-1.390222000	-0.338505000
Ag	0.000000000	0.000000000	4.030835000
Ag	0.000000000	-2.048856000	2.087122000
Ag	0.000000000	2.445446000	-2.572570000
Ag	0.000000000	3.773090000	-0.102729000
Ag	1.392831000	0.000000000	-2.765250000
Ag	0.000000000	-3.773090000	-0.102729000
Ag	0.000000000	-2.445446000	-2.572570000
Ag	-1.392831000	0.000000000	-2.765250000