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

Supplementary Information

Comment on "Structural characterization, reactivity and vibrational properties of silver clusters: a new global minimum for Ag16" by P. L. Rodríguez-Kessler, A. R. Rodríguez-Domínguez, D, MacLeod Carey and A. Muñoz-Castro, Phys. Chem. Chem. Phys., 2020, 22, 27255, DOI: D0CP04018E

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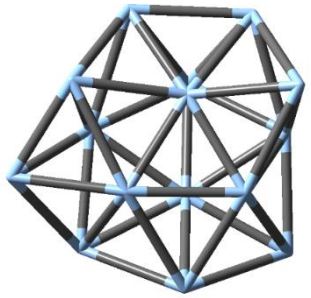
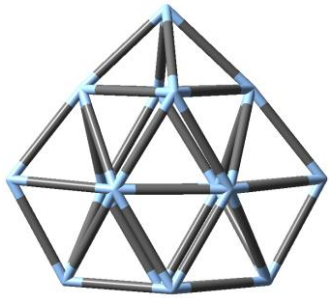
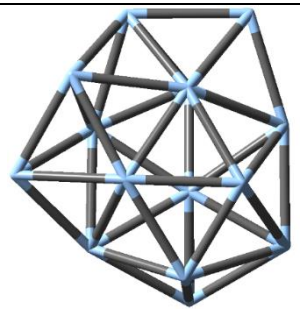
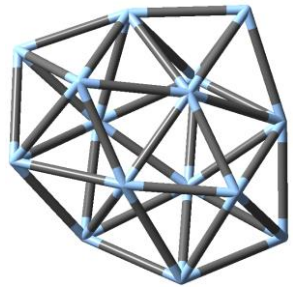
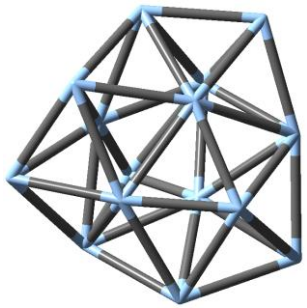
Table S1. Geometries, Cartesian coordinates and total energies of optimized Ag_{15} lower-lying isomers (PW91/cc-pVDZ-PP).

Structure	Cartesian coordinates (angstrom)				Energy (Hartree)
 **15-1,** C_1, ^{2}A	47	1.351847000	3.120690000	0.408251000	Zero-point correction= 0.008681
	47	-1.114309000	-1.055441000	-2.056970000	Thermal correction to Energy= 0.040458
	47	0.191211000	1.258125000	-1.274935000	Thermal correction to Enthalpy= 0.041402
	47	1.524353000	-1.175668000	-1.167923000	Thermal correction to Gibbs Free Energy= -0.069075
	47	3.860983000	-1.064021000	0.411598000	Sum of electronic and zero-point Energies= -2205.876915
	47	1.660777000	0.403667000	1.344950000	Sum of electronic and thermal Energies= -2205.845138
	47	-0.706917000	-0.989192000	0.854417000	Sum of electronic and thermal Enthalpies= -2205.844194
	47	1.638842000	-2.528762000	1.218002000	Sum of electronic and thermal Free Energies= -2205.954671
	47	-0.848666000	1.678195000	1.453276000	
	47	-0.501995000	-3.351984000	-0.477939000	
	47	-3.062317000	-1.941694000	-0.283989000	
	47	3.006819000	1.253101000	-0.946636000	
	47	-2.558738000	0.928873000	-0.718499000	
	47	-3.110757000	-0.030944000	1.830357000	
	47	-1.331132000	3.495057000	-0.593959000	
 **15-2**, C_{2v}, ^{2}B$_1$	47	0.000000000	3.772961000	-0.102661000	Zero-point correction= 0.008883
	47	1.436131000	-1.390156000	-0.338879000	Thermal correction to Energy= 0.040480
	47	1.436131000	1.390156000	-0.338879000	Thermal correction to Enthalpy=0.041424
	47	1.906206000	0.000000000	2.015745000	Thermal correction to Gibbs Free Energy= -0.067263
	47	0.000000000	2.048371000	2.087309000	Sum of electronic and zero-point Energies= -2205.876625
	47	1.393033000	0.000000000	-2.765229000	Sum of electronic and thermal Energies= -2205.845028
	47	-1.436131000	1.390156000	-0.338879000	Sum of electronic and thermal Enthalpies= -2205.844084
	47	-1.436131000	-1.390156000	-0.338879000	Sum of electronic and thermal Free Energies= -2205.952771
	47	-1.906206000	0.000000000	2.015745000	
	47	-1.393033000	0.000000000	-2.765229000	
	47	0.000000000	2.445841000	-2.573068000	
	47	0.000000000	-2.445841000	-2.573068000	
	47	0.000000000	-2.048371000	2.087309000	
	47	0.000000000	0.000000000	4.031324000	
	47	0.000000000	-3.772961000	-0.102661000	

 **15-3**, C_1, ^{2}A	47	-0.376265000	1.466385000	1.404506000	Zero-point correction= 0.008649
	47	3.585201000	0.212948000	-0.586008000	Thermal correction to Energy= 0.040455
	47	1.535487000	-1.223902000	-1.784044000	Thermal correction to Enthalpy= 0.041399
	47	-0.956880000	-0.529815000	-0.848556000	Thermal correction to Gibbs Free Energy= -0.069217
	47	0.978646000	1.428725000	-1.255953000	Sum of electronic and zero-point Energies= -2205.875253
	47	1.525376000	-0.541629000	1.056984000	Sum of electronic and thermal Energies= -2205.843448
	47	-0.985895000	-1.205949000	2.031232000	Sum of electronic and thermal Enthalpies= -2205.842504
	47	3.042052000	-2.631205000	0.069661000	Sum of electronic and thermal Free Energies= -2205.953119
	47	0.202173000	-2.932044000	0.110092000	
	47	0.222937000	3.812586000	0.004400000	
	47	2.360223000	2.203400000	1.004081000	
	47	-1.865226000	2.118812000	-0.889563000	
	47	-2.688502000	-2.404257000	0.123607000	
	47	-2.984180000	0.403819000	1.081697000	
	47	-3.595148000	-0.177874000	-1.522137000	
 **15-4**, C_s, ^{2}A’	47	0.145251000	1.630084000	2.376304000	Zero-point correction= 0.008620
	47	1.559920000	1.320603000	0.000000000	Thermal correction to Energy= 0.040455
	47	-2.106757000	-0.102895000	2.338979000	Thermal correction to Enthalpy= 0.041400
	47	-1.882618000	-1.643067000	0.000000000	Thermal correction to Gibbs Free Energy= -0.069506
	47	0.441537000	-1.151724000	-1.369232000	Sum of electronic and zero-point Energies= -2205.873827
	47	0.441537000	-1.151724000	1.369232000	Sum of electronic and thermal Energies= -2205.841992
	47	-1.238077000	1.225824000	0.000000000	Sum of electronic and thermal Enthalpies= -2205.841047
	47	0.145251000	1.630084000	-2.376304000	Sum of electronic and thermal Free Energies= -2205.951953
	47	-3.839763000	0.300079000	0.000000000	
	47	-2.106757000	-0.102895000	-2.338979000	
	47	2.560291000	0.170375000	2.540022000	
	47	0.170573000	-0.639333000	4.016061000	
	47	2.978749000	-1.016451000	0.000000000	
	47	0.170573000	-0.639333000	-4.016061000	
	47	2.560291000	0.170375000	-2.540022000	



15-5, C_1, ^{2}A

47	-2.427943000	-1.593925000	0.874273000
47	3.440274000	1.745939000	-0.072146000
47	-2.016334000	3.304336000	0.062780000
47	0.855381000	2.872016000	-0.015728000
47	3.244886000	-1.087500000	0.144662000
47	-0.971032000	0.874309000	0.808137000
47	0.475309000	-1.695609000	0.868270000
47	-1.094775000	-1.035527000	-1.539461000
47	-0.902511000	1.694611000	-1.893831000
47	1.635280000	0.683127000	1.729926000
47	1.400401000	0.344192000	-1.316329000
47	1.443095000	-2.499051000	-1.508650000
47	-3.269968000	0.689769000	-0.658167000
47	-0.811320000	-0.676389000	3.043607000
47	-1.000744000	-3.620297000	-0.527343000

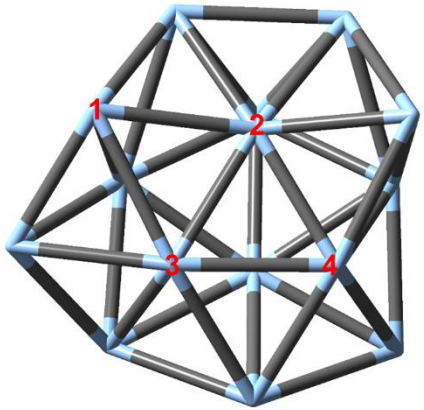
Zero-point correction= 0.008570
Thermal correction to Energy= 0.040450
Thermal correction to Enthalpy= 0.041394
Thermal correction to Gibbs Free Energy= -0.069862
Sum of electronic and zero-point Energies= -2205.867994
Sum of electronic and thermal Energies= -2205.836114
Sum of electronic and thermal Enthalpies= -2205.835170
Sum of electronic and thermal Free Energies= -2205.946426

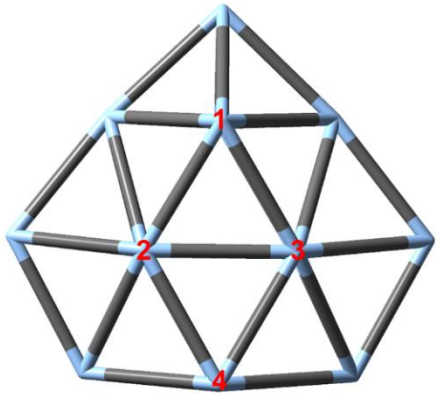
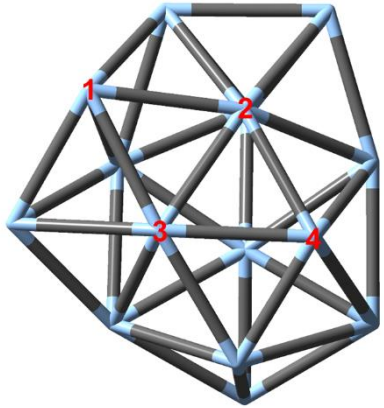
Table S2. Some representative bond distances (angstrom) and angles (degree) in low-lying Ag_{15} isomers computed with different functionals.

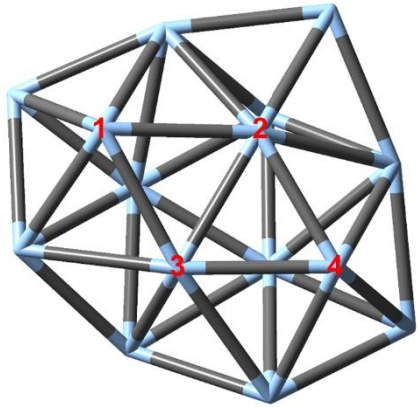
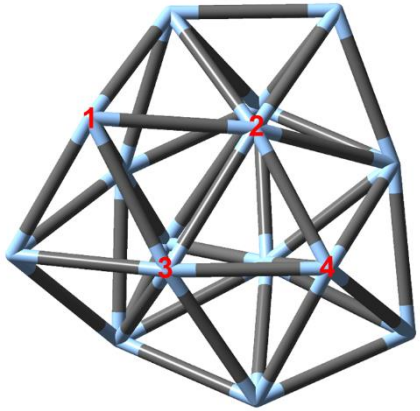
A comparison with previous calculated results by Rodríguez-Kessler *et al.* (**15-1 - 15-4**) and by Dixon *et al.* (**15-5**) shows that these structural parameters are marginally changed with respect to the DFT-functional employed, and comparable to previous calculated results reported in the literature:

P. L. Rodríguez-Kessler, A. R. Rodríguez-Domínguez, D. M. Carey and A. Muñoz-Castro, *Phys. Chem. Chem. Phys.*, 2020, **22**, 27255-27262.
R. R. Persaud, M. Chen and D. A. Dixon, *J. Phys. Chem. A*, 2020, **124**, 1775-1786.

The variations amount to at most 0.08 Å for bond distances and 2° for bond angles.

Structure	Parameter	PW91	PBE	TPSS	LC-BLYP	M06	B3LYP	Previous calculations
 **15-1,** C_1, ^{2}A	Ag1-Ag2	2.829	2.840	2.808	2.790	2.889	2.908	2.829
	Ag1-Ag3	2.935	2.860	2.883	2.852	2.999	2.878	2.935
	Ag2-Ag4	2.737	2.777	2.718	2.716	2.791	2.814	2.737
	Ag3-Ag4	2.817	2.796	2.804	2.775	2.871	2.821	2.817
	∠Ag2-Ag3-Ag4	58°	59°	58°	58°	58°	60°	58°

 **15-2**, C_{2v}, $^2B_1$	Ag1-Ag2	2.774	2.779	2.755	2.760	2.824	2.817	2.802
	Ag1-Ag3	2.774	2.779	2.755	2.760	2.824	2.817	2.802
	Ag2-Ag4	2.797	2.801	2.769	2.751	2.852	2.848	2.792
	Ag3-Ag4	2.797	2.801	2.769	2.751	2.852	2.848	2.792
	∠Ag1-Ag2-Ag3	60°	60°	60°	60°	59°	59°	60°
 **15-3**, C_1, ^2A	Ag1-Ag2	2.869	2.874	2.826	2.838	2.924	2.926	2.866
	Ag1-Ag3	2.862	2.868	2.847	2.834	2.922	2.918	2.810
	Ag2-Ag4	2.774	2.781	2.800	2.775	2.827	2.824	2.793
	Ag3-Ag4	2.812	2.819	2.759	2.784	2.865	2.833	2.816
	∠Ag2-Ag3-Ag4	59°	59°	61°	60°	59°	59°	59°
	Ag1-Ag2	2.779	2.785	2.759	2.763	2.831	2.831	2.796
	Ag1-Ag3	2.783	2.790	2.773	2.753	2.836	2.813	2.793

 **15-4**, C_s, ^{2}A’	Ag2-Ag4	2.779	2.785	2.759	2.763	2.831	2.831	2.796
	Ag3-Ag4	2.783	2.790	2.773	2.753	2.836	2.813	2.793
	∠Ag2-Ag3-Ag4	59°	59°	59°	59°	59°	60°	60°
 **15-5**, C_1, ^{2}A	Ag1-Ag2	2.850	2.857	2.821	2.783	2.916	2.925	2.915
	Ag1-Ag3	2.930	2.938	2.899	2.871	2.999	3.011	2.994
	Ag2-Ag4	2.731	2.737	2.720	2.737	2.783	2.764	2.754
	Ag3-Ag4	2.760	2.768	2.753	2.722	2.807	2.782	2.769
	∠Ag2-Ag3-Ag4	58°	58°	58°	58°	57°	58°	58°