Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Theoretical modeling of optical properties of Ag_8 and Ag_{14} silver clusters embedded in LTA sodalite zeolite cavity

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Cartesian Coordinate (in Angstrom) of $[Ag_{14}(Al_{12}Si_{12}H_{24}O_{36})]^{p-}$ cluster

optimized at B3LYP/LANL2DZ

$[Ag_{14}(Al_{12}Si_{12}H_{24}O_{36})]$:

O	1.378165000	1.378169000	4.136062000
O	4.136107000	1.378140000	1.378139000
O	1.378167000	4.136063000	1.378170000
O	3.665272000	0.000000000	3.665272000
O	1.378165000	-1.378169000	4.136062000
O	1.378167000	-4.136063000	1.378170000
O	4.136107000	-1.378140000	1.378139000
O	0.000000000	3.665267000	3.665267000
O	-1.378165000	1.378169000	4.136062000
O	-1.378167000	4.136063000	1.378170000
O	-4.136107000	1.378140000	1.378139000
O	0.000000000	-3.665267000	3.665267000
O	-3.665272000	0.000000000	3.665272000
O	-1.378165000	-1.378169000	4.136062000
O	-4.136107000	-1.378140000	1.378139000
O	-1.378167000	-4.136063000	1.378170000
O	3.665272000	3.665272000	0.000000000
O	1.378165000	1.378169000	-4.136062000
O	1.378167000	4.136063000	-1.378170000
O	4.136107000	1.378140000	-1.378139000
O	3.665272000	0.000000000	-3.665272000
O	3.665272000	-3.665272000	0.000000000
O	1.378165000	-1.378169000	-4.136062000
O	4.136107000	-1.378140000	-1.378139000
O	1.378167000	-4.136063000	-1.378170000
O	0.000000000	3.665267000	-3.665267000
O	-3.665272000	3.665272000	0.000000000

O	-1.378165000	1.378169000	-4.136062000
O	-4.136107000	1.378140000	-1.378139000
O	-1.378167000	4.136063000	-1.378170000
O	-3.665272000	0.000000000	-3.665272000
O	-1.378165000	-1.378169000	-4.136062000
O	0.000000000	-3.665267000	-3.665267000
O	-3.665272000	-3.665272000	0.000000000
O	-1.378167000	-4.136063000	-1.378170000
O	-4.136107000	-1.378140000	-1.378139000
Si	-2.195957000	-4.519480000	0.000000000
H	-2.838461000	-5.841479000	0.000000000
H	0.000000000	-5.913433000	2.873429000
Si	2.195957000	-4.519480000	0.000000000
H	2.838461000	-5.841479000	0.000000000
H	0.000000000	-5.913433000	-2.873429000
H	-5.894564000	-2.864251000	0.000000000
Si	-4.519439000	0.000000000	2.195938000
H	-5.841476000	0.000000000	2.838465000
Si	0.000000000	-2.195944000	4.519486000
H	0.000000000	-2.838467000	5.841477000
H	5.894564000	-2.864251000	0.000000000
H	2.873425000	0.000000000	5.913433000
Si	4.519439000	0.000000000	2.195938000
H	5.841476000	0.000000000	2.838465000
Si	4.519439000	0.000000000	-2.195938000
H	5.841476000	0.000000000	-2.838465000
H	5.894564000	2.864251000	0.000000000
Si	2.195957000	4.519480000	0.000000000
H	2.838461000	5.841479000	0.000000000
H	0.000000000	5.913433000	2.873429000
H	0.000000000	5.913433000	-2.873429000
Si	-2.195957000	4.519480000	0.000000000
H	-2.838461000	5.841479000	0.000000000
Si	0.000000000	2.195944000	-4.519486000
H	0.000000000	2.838467000	-5.841477000
Si	0.000000000	2.195944000	4.519486000
H	0.000000000	2.838467000	5.841477000
H	2.873425000	0.000000000	-5.913433000
H	-2.873425000	0.000000000	-5.913433000
H	-5.894564000	2.864251000	0.000000000
Si	-4.519439000	0.000000000	-2.195938000
H	-5.841476000	0.000000000	-2.838465000
Si	0.000000000	-2.195944000	-4.519486000
H	0.000000000	-2.838467000	-5.841477000
H	-2.873425000	0.000000000	5.913433000
Al	4.519438000	-2.195936000	0.000000000
Al	4.519438000	2.195936000	0.000000000
Al	0.000000000	-4.519490000	2.195939000
Al	2.195959000	0.000000000	4.519476000
Al	0.000000000	-4.519490000	-2.195939000
Al	-2.195959000	0.000000000	4.519476000

Al	0.000000000	4.519490000	2.195939000
Al	-4.519438000	2.195936000	0.000000000
Al	-4.519438000	-2.195936000	0.000000000
Al	-2.195959000	0.000000000	-4.519476000
Al	0.000000000	4.519490000	-2.195939000
Al	2.195959000	0.000000000	-4.519476000
Ag	2.838413000	2.838135000	2.837877000
Ag	-2.838413000	2.838135000	-2.837877000
Ag	2.838413000	-2.838135000	-2.837877000
Ag	-2.838413000	-2.838135000	2.837877000
Ag	2.838413000	2.838135000	-2.837877000
Ag	-2.838413000	2.838135000	2.837877000
Ag	2.838413000	-2.838135000	2.837877000
Ag	-2.838413000	-2.838135000	-2.837877000
Ag	2.107957000	0.000000000	0.000000000
Ag	0.000000000	0.000000000	2.107297000
Ag	0.000000000	2.107455000	0.000000000
Ag	-2.107957000	0.000000000	0.000000000
Ag	0.000000000	0.000000000	-2.107297000
Ag	0.000000000	-2.107455000	0.000000000

$[Ag_{14}(Al_{12}Si_{12}H_{24}O_{36})]^{2-}$:

O	-1.377985000	4.136415000	1.377986000
O	-4.136425000	1.377992000	1.377991000
O	-1.377994000	1.377994000	4.136424000
O	-3.665283000	3.665282000	0.000000000
O	-1.377985000	4.136415000	-1.377986000
O	-1.377994000	1.377994000	-4.136424000
O	-4.136425000	1.377992000	-1.377991000
O	0.000000000	3.665281000	3.665280000
O	1.377985000	4.136415000	1.377986000
O	1.377994000	1.377994000	4.136424000
O	4.136425000	1.377992000	1.377991000
O	0.000000000	3.665281000	-3.665280000
O	3.665283000	3.665282000	0.000000000
O	1.377985000	4.136415000	-1.377986000
O	4.136425000	1.377992000	-1.377991000
O	1.377994000	1.377994000	-4.136424000
O	-3.665283000	0.000000000	3.665281000
O	-1.377985000	-4.136415000	1.377986000
O	-1.377994000	-1.377994000	4.136424000
O	-4.136425000	-1.377992000	1.377991000
O	-3.665283000	-3.665282000	0.000000000
O	-3.665283000	0.000000000	-3.665281000
O	-1.377985000	-4.136415000	-1.377986000
O	-4.136425000	-1.377992000	-1.377991000
O	-1.377994000	-1.377994000	-4.136424000
O	0.000000000	-3.665281000	3.665280000

O	3.665283000	0.000000000	3.665281000
O	1.377985000	-4.136415000	1.377986000
O	4.136425000	-1.377992000	1.377991000
O	1.377994000	-1.377994000	4.136424000
O	3.665283000	-3.665282000	0.000000000
O	1.377985000	-4.136415000	-1.377986000
O	0.000000000	-3.665281000	-3.665280000
O	3.665283000	0.000000000	-3.665281000
O	1.377994000	-1.377994000	-4.136424000
O	4.136425000	-1.377992000	-1.377991000
Si	2.195977000	0.000000000	-4.519308000
H	2.838442000	0.000000000	-5.841489000
H	0.000000000	2.873406000	-5.913444000
Si	-2.195977000	0.000000000	-4.519308000
H	-2.838442000	0.000000000	-5.841489000
H	0.000000000	-2.873406000	-5.913444000
H	5.894576000	0.000000000	-2.864230000
Si	4.519304000	2.195973000	0.000000000
H	5.841488000	2.838444000	0.000000000
Si	0.000000000	4.519308000	-2.195973000
H	0.000000000	5.841488000	-2.838444000
H	-5.894576000	0.000000000	-2.864230000
H	-2.873408000	5.913443000	0.000000000
Si	-4.519304000	2.195973000	0.000000000
H	-5.841488000	2.838444000	0.000000000
Si	-4.519304000	-2.195973000	0.000000000
H	-5.841488000	-2.838444000	0.000000000
H	-5.894576000	0.000000000	2.864230000
Si	-2.195977000	0.000000000	4.519308000
H	-2.838442000	0.000000000	5.841489000
H	0.000000000	2.873406000	5.913444000
H	0.000000000	-2.873406000	5.913444000
Si	2.195977000	0.000000000	4.519308000
H	2.838442000	0.000000000	5.841489000
Si	0.000000000	-4.519308000	2.195973000
H	0.000000000	-5.841488000	2.838444000
Si	0.000000000	4.519308000	2.195973000
H	0.000000000	5.841488000	2.838444000
H	-2.873408000	-5.913443000	0.000000000
H	2.873408000	-5.913443000	0.000000000
H	5.894576000	0.000000000	2.864230000
Si	4.519304000	-2.195973000	0.000000000
H	5.841488000	-2.838444000	0.000000000
Si	0.000000000	-4.519308000	-2.195973000
H	0.000000000	-5.841488000	-2.838444000
H	2.873408000	5.913443000	0.000000000
Al	-4.519303000	0.000000000	-2.195971000
Al	-4.519303000	0.000000000	2.195971000
Al	0.000000000	2.195976000	-4.519310000
Al	-2.195975000	4.519307000	0.000000000
Al	0.000000000	-2.195976000	-4.519310000

Al	2.195975000	4.519307000	0.000000000
Al	0.000000000	2.195976000	4.519310000
Al	4.519303000	0.000000000	2.195971000
Al	4.519303000	0.000000000	-2.195971000
Al	2.195975000	-4.519307000	0.000000000
Al	0.000000000	-2.195976000	4.519310000
Al	-2.195975000	-4.519307000	0.000000000
Ag	-2.695167000	2.667953000	2.671933000
Ag	2.695167000	-2.667953000	2.671933000
Ag	-2.695167000	-2.667953000	-2.671933000
Ag	2.695167000	2.667953000	-2.671933000
Ag	-2.695167000	-2.667953000	2.671933000
Ag	2.695167000	2.667953000	2.671933000
Ag	-2.695167000	2.667953000	-2.671933000
Ag	2.695167000	-2.667953000	-2.671933000
Ag	-2.042842000	0.000000000	0.000000000
Ag	0.000000000	2.045021000	0.000000000
Ag	0.000000000	0.000000000	1.973973000
Ag	2.042842000	0.000000000	0.000000000
Ag	0.000000000	-2.045021000	0.000000000
Ag	0.000000000	0.000000000	-1.973973000

$[Ag_{14}(Al_{12}Si_{12}H_{24}O_{36})]^{4-}$:

O	-4.136417000	1.377996000	1.377996000
O	-1.377992000	1.377992000	4.136411000
O	-1.377996000	4.136417000	1.377996000
O	-3.665276000	0.000000000	3.665276000
O	-4.136417000	-1.377996000	1.377996000
O	-1.377996000	-4.136417000	1.377996000
O	-1.377992000	-1.377992000	4.136411000
O	-3.665276000	3.665276000	0.000000000
O	-4.136417000	1.377996000	-1.377996000
O	-1.377996000	4.136417000	-1.377996000
O	-1.377992000	1.377992000	-4.136411000
O	-3.665276000	-3.665276000	0.000000000
O	-3.665276000	0.000000000	-3.665276000
O	-4.136417000	-1.377996000	-1.377996000
O	-1.377992000	-1.377992000	-4.136411000
O	-1.377996000	-4.136417000	-1.377996000
O	0.000000000	3.665276000	3.665276000
O	4.136417000	1.377996000	1.377996000
O	1.377996000	4.136417000	1.377996000
O	1.377992000	1.377992000	4.136411000
O	3.665276000	0.000000000	3.665276000
O	0.000000000	-3.665276000	3.665276000
O	4.136417000	-1.377996000	1.377996000
O	1.377992000	-1.377992000	4.136411000

O	1.377996000	-4.136417000	1.377996000
O	3.665276000	3.665276000	0.000000000
O	0.000000000	3.665276000	-3.665276000
O	4.136417000	1.377996000	-1.377996000
O	1.377992000	1.377992000	-4.136411000
O	1.377996000	4.136417000	-1.377996000
O	3.665276000	0.000000000	-3.665276000
O	4.136417000	-1.377996000	-1.377996000
O	3.665276000	-3.665276000	0.000000000
O	0.000000000	-3.665276000	-3.665276000
O	1.377996000	-4.136417000	-1.377996000
O	1.377992000	-1.377992000	-4.136411000
Si	0.000000000	-4.519336000	-2.195975000
H	0.000000000	-5.841487000	-2.838446000
H	-2.873410000	-5.913442000	0.000000000
Si	0.000000000	-4.519336000	2.195975000
H	0.000000000	-5.841487000	2.838446000
H	2.873410000	-5.913442000	0.000000000
H	0.000000000	-2.864233000	-5.894575000
Si	-2.195979000	0.000000000	-4.519342000
H	-2.838447000	0.000000000	-5.841487000
Si	-4.519335000	-2.195974000	0.000000000
H	-5.841487000	-2.838446000	0.000000000
H	0.000000000	-2.864233000	5.894575000
H	-5.913442000	0.000000000	2.873410000
Si	-2.195979000	0.000000000	4.519342000
H	-2.838447000	0.000000000	5.841487000
Si	2.195979000	0.000000000	4.519342000
H	2.838447000	0.000000000	5.841487000
H	0.000000000	2.864233000	5.894575000
Si	0.000000000	4.519336000	2.195975000
H	0.000000000	5.841487000	2.838446000
H	-2.873410000	5.913442000	0.000000000
H	2.873410000	5.913442000	0.000000000
Si	0.000000000	4.519336000	-2.195975000
H	0.000000000	5.841487000	-2.838446000
Si	4.519335000	2.195974000	0.000000000
H	5.841487000	2.838446000	0.000000000
Si	-4.519335000	2.195974000	0.000000000
H	-5.841487000	2.838446000	0.000000000
H	5.913442000	0.000000000	2.873410000
H	5.913442000	0.000000000	-2.873410000
H	0.000000000	2.864233000	-5.894575000
Si	2.195979000	0.000000000	-4.519342000
H	2.838447000	0.000000000	-5.841487000
Si	4.519335000	-2.195974000	0.000000000

H	5.841487000	-2.838446000	0.000000000
H	-5.913442000	0.000000000	-2.873410000
Al	0.000000000	-2.195979000	4.519342000
Al	0.000000000	2.195979000	4.519342000
Al	-2.195975000	-4.519334000	0.000000000
Al	-4.519335000	0.000000000	2.195976000
Al	2.195975000	-4.519334000	0.000000000
Al	-4.519335000	0.000000000	-2.195976000
Al	-2.195975000	4.519334000	0.000000000
Al	0.000000000	2.195979000	-4.519342000
Al	0.000000000	-2.195979000	-4.519342000
Al	4.519335000	0.000000000	-2.195976000
Al	2.195975000	4.519334000	0.000000000
Al	4.519335000	0.000000000	2.195976000
Ag	-2.083363000	2.083412000	2.082145000
Ag	2.083363000	2.083412000	-2.082145000
Ag	2.083363000	-2.083412000	2.082145000
Ag	-2.083363000	-2.083412000	-2.082145000
Ag	2.083363000	2.083412000	2.082145000
Ag	-2.083363000	2.083412000	-2.082145000
Ag	-2.083363000	-2.083412000	2.082145000
Ag	2.083363000	-2.083412000	-2.082145000
Ag	0.000000000	0.000000000	1.865657000
Ag	-2.057010000	0.000000000	0.000000000
Ag	0.000000000	2.056904000	0.000000000
Ag	0.000000000	0.000000000	-1.865657000
Ag	2.057010000	0.000000000	0.000000000
Ag	0.000000000	-2.056904000	0.000000000

$[Ag_{14}(Al_{12}Si_{12}H_{24}O_{36})]^{6-}$:

O	-4.136354000	1.378011000	1.378003000
O	-1.378010000	1.378010000	4.136383000
O	-1.378016000	4.136358000	1.378008000
O	-3.665273000	0.000000000	3.665274000
O	-4.136354000	-1.378011000	1.378003000
O	-1.378016000	-4.136358000	1.378008000
O	-1.378010000	-1.378010000	4.136383000
O	-3.665271000	3.665272000	0.000000000
O	-4.136354000	1.378011000	-1.378003000
O	-1.378016000	4.136358000	-1.378008000
O	-1.378010000	1.378010000	-4.136383000
O	-3.665271000	-3.665272000	0.000000000
O	-3.665273000	0.000000000	-3.665274000
O	-4.136354000	-1.378011000	-1.378003000
O	-1.378010000	-1.378010000	-4.136383000

O	-1.378016000	-4.136358000	-1.378008000
O	0.000000000	3.665274000	3.665276000
O	4.136354000	1.378011000	1.378003000
O	1.378016000	4.136358000	1.378008000
O	1.378010000	1.378010000	4.136383000
O	3.665273000	0.000000000	3.665274000
O	0.000000000	-3.665274000	3.665276000
O	4.136354000	-1.378011000	1.378003000
O	1.378010000	-1.378010000	4.136383000
O	1.378016000	-4.136358000	1.378008000
O	3.665271000	3.665272000	0.000000000
O	0.000000000	3.665274000	-3.665276000
O	4.136354000	1.378011000	-1.378003000
O	1.378010000	1.378010000	-4.136383000
O	1.378016000	4.136358000	-1.378008000
O	3.665273000	0.000000000	-3.665274000
O	4.136354000	-1.378011000	-1.378003000
O	3.665271000	-3.665272000	0.000000000
O	0.000000000	-3.665274000	-3.665276000
O	1.378016000	-4.136358000	-1.378008000
O	1.378010000	-1.378010000	-4.136383000
Si	0.000000000	-4.519364000	-2.195968000
H	0.000000000	-5.841484000	-2.838451000
H	-2.873419000	-5.913438000	0.000000000
Si	0.000000000	-4.519364000	2.195968000
H	0.000000000	-5.841484000	2.838451000
H	2.873419000	-5.913438000	0.000000000
H	0.000000000	-2.864234000	-5.894573000
Si	-2.195968000	0.000000000	-4.519348000
H	-2.838448000	0.000000000	-5.841485000
Si	-4.519378000	-2.195954000	0.000000000
H	-5.841482000	-2.838457000	0.000000000
H	0.000000000	-2.864234000	5.894573000
H	-5.913439000	0.000000000	2.873414000
Si	-2.195968000	0.000000000	4.519348000
H	-2.838448000	0.000000000	5.841485000
Si	2.195968000	0.000000000	4.519348000
H	2.838448000	0.000000000	5.841485000
H	0.000000000	2.864234000	5.894573000
Si	0.000000000	4.519364000	2.195968000
H	0.000000000	5.841484000	2.838451000
H	-2.873419000	5.913438000	0.000000000
H	2.873419000	5.913438000	0.000000000
Si	0.000000000	4.519364000	-2.195968000
H	0.000000000	5.841484000	-2.838451000
Si	4.519378000	2.195954000	0.000000000

H	5.841482000	2.838457000	0.000000000
Si	-4.519378000	2.195954000	0.000000000
H	-5.841482000	2.838457000	0.000000000
H	5.913439000	0.000000000	2.873414000
H	5.913439000	0.000000000	-2.873414000
H	0.000000000	2.864234000	-5.894573000
Si	2.195968000	0.000000000	-4.519348000
H	2.838448000	0.000000000	-5.841485000
Si	4.519378000	-2.195954000	0.000000000
H	5.841482000	-2.838457000	0.000000000
H	-5.913439000	0.000000000	-2.873414000
Al	0.000000000	-2.195965000	4.519345000
Al	0.000000000	2.195965000	4.519345000
Al	-2.195954000	-4.519375000	0.000000000
Al	-4.519370000	0.000000000	2.195973000
Al	2.195954000	-4.519375000	0.000000000
Al	-4.519370000	0.000000000	-2.195973000
Al	-2.195954000	4.519375000	0.000000000
Al	0.000000000	2.195965000	-4.519345000
Al	0.000000000	-2.195965000	-4.519345000
Al	4.519370000	0.000000000	-2.195973000
Al	2.195954000	4.519375000	0.000000000
Al	4.519370000	0.000000000	2.195973000
Ag	-1.989327000	1.989472000	1.989536000
Ag	1.989327000	1.989472000	-1.989536000
Ag	1.989327000	-1.989472000	1.989536000
Ag	-1.989327000	-1.989472000	-1.989536000
Ag	1.989327000	1.989472000	1.989536000
Ag	-1.989327000	1.989472000	-1.989536000
Ag	-1.989327000	-1.989472000	1.989536000
Ag	1.989327000	-1.989472000	-1.989536000
Ag	0.000000000	0.000000000	1.974163000
Ag	-1.973507000	0.000000000	0.000000000
Ag	0.000000000	1.973254000	0.000000000
Ag	0.000000000	0.000000000	-1.974163000
Ag	1.973507000	0.000000000	0.000000000
Ag	0.000000000	-1.973254000	0.000000000

$[Ag_{14}(Al_{12}Si_{12}H_{24}O_{36})]^{8-}$:

O	-4.136896000	-1.373383000	-1.380897000
O	-1.378614000	-1.368641000	-4.139268000
O	-1.379727000	-4.132829000	-1.386804000
O	-3.665301000	0.009302000	-3.665228000
O	-4.135651000	1.382679000	-1.375072000
O	-1.376383000	4.139723000	-1.369231000

O	-1.377518000	1.387406000	-4.133284000
O	-3.666771000	-3.663761000	-0.007768000
O	-4.136757000	-1.379289000	1.375150000
O	-1.379749000	-4.138594000	1.369255000
O	-1.378576000	-1.386277000	4.133307000
O	-3.663768000	3.666765000	0.007837000
O	-3.665239000	-0.006298000	3.665297000
O	-4.135743000	1.376772000	1.380975000
O	-1.377414000	1.369769000	4.139292000
O	-1.376314000	4.133957000	1.386828000
O	-0.001534000	-3.657458000	-3.673064000
O	4.135629000	-1.376812000	-1.381016000
O	1.376359000	-4.133856000	-1.386866000
O	1.377448000	-1.369796000	-4.139176000
O	3.665239000	0.006302000	-3.665297000
O	0.001473000	3.673063000	-3.657460000
O	4.136872000	1.379250000	-1.375109000
O	1.378544000	1.386251000	-4.133427000
O	1.379703000	4.138695000	-1.369219000
O	3.663768000	-3.666765000	-0.007836000
O	-0.001469000	-3.673063000	3.657460000
O	4.135767000	-1.382639000	1.375030000
O	1.377486000	-1.387379000	4.133400000
O	1.376337000	-4.139823000	1.369192000
O	3.665300000	-0.009306000	3.665227000
O	4.136780000	1.373423000	1.380938000
O	3.666771000	3.663761000	0.007767000
O	0.001531000	3.657458000	3.673064000
O	1.379772000	4.132728000	1.386839000
O	1.378647000	1.368668000	4.139149000
Si	0.001869000	4.514724000	2.205558000
H	0.002420000	5.835423000	2.850890000
H	-2.871006000	5.914596000	0.012614000
Si	0.001835000	4.524072000	-2.186318000
H	0.002369000	5.847508000	-2.826022000
H	2.875852000	5.912242000	0.012562000
H	0.001225000	2.851691000	5.900651000
Si	-2.195905000	-0.008723000	4.519404000
H	-2.838410000	-0.011273000	5.841493000
Si	-4.518525000	2.197777000	0.004717000
H	-5.840314000	2.840856000	0.006094000
H	0.001122000	2.876786000	-5.888457000
H	-5.913457000	0.008542000	-2.873364000
Si	-2.195982000	0.010522000	-4.519365000
H	-2.838510000	0.013600000	-5.841439000
Si	2.195906000	0.008719000	-4.519406000

H	2.838409000	0.011270000	-5.841493000
H	-0.001223000	-2.851691000	-5.900651000
Si	-0.001872000	-4.514723000	-2.205559000
H	-0.002416000	-5.835423000	-2.850891000
H	-2.875851000	-5.912242000	-0.012560000
H	2.871006000	-5.914596000	-0.012616000
Si	-0.001833000	-4.524072000	2.186317000
H	-0.002371000	-5.847508000	2.826021000
Si	4.518525000	-2.197777000	-0.004718000
H	5.840313000	-2.840856000	-0.006100000
Si	-4.520324000	-2.194073000	-0.004631000
H	-5.842639000	-2.836068000	-0.005985000
H	5.913409000	0.003692000	-2.873474000
H	5.913458000	-0.008537000	2.873363000
H	-0.001125000	-2.876786000	5.888457000
Si	2.195982000	-0.010518000	4.519364000
H	2.838510000	-0.013596000	5.841439000
Si	4.520324000	2.194073000	0.004633000
H	5.842640000	2.836069000	0.005990000
H	-5.913410000	-0.003696000	2.873474000
Al	0.000858000	2.205561000	-4.514713000
Al	-0.000935000	-2.186320000	-4.524062000
Al	-2.194074000	4.520302000	0.009644000
Al	-4.519435000	0.006527000	-2.195901000
Al	2.197778000	4.518503000	0.009596000
Al	-4.519398000	-0.002822000	2.195986000
Al	-2.197778000	-4.518503000	-0.009603000
Al	-0.000865000	-2.205561000	4.514713000
Al	0.000940000	2.186320000	4.524062000
Al	4.519434000	-0.006527000	2.195900000
Al	2.194074000	-4.520302000	-0.009638000
Al	4.519398000	0.002822000	-2.195986000
Ag	-1.942291000	-1.929236000	-1.935885000
Ag	1.940733000	-1.938904000	1.927782000
Ag	1.942276000	1.937335000	-1.927810000
Ag	-1.940701000	1.930804000	1.935910000
Ag	2.719431000	-2.710345000	-2.713943000
Ag	-2.721684000	-2.719639000	2.702466000
Ag	-2.719507000	2.721853000	-2.702411000
Ag	2.721698000	2.708132000	2.713902000
Ag	-0.000111000	0.004212000	-1.971569000
Ag	-1.962949000	0.000813000	-0.000015000
Ag	-0.000705000	-1.965195000	-0.004168000
Ag	-0.000087000	-0.004203000	1.971566000
Ag	1.962962000	-0.000822000	-0.000042000
Ag	0.000936000	1.965194000	0.004222000

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Cartesian Coordinate (in Angstrom) of Ag_{14}^{6+}@ZA cluster

optimized at B3LYP/LANL2DZ

[$Ag_{14}(Al_6Si_{18}H_{24}O_{36})$]:

O	-4.231491000	1.378043000	-1.050151000
O	-3.378106000	1.378013000	2.756285000
O	-1.901562000	4.136340000	0.426344000
O	-5.057911000	0.000007000	1.134002000
O	-4.231496000	-1.378001000	-1.050152000
O	-1.901611000	-4.136360000	0.426322000
O	-3.378086000	-1.377990000	2.756252000
O	-3.095944000	3.665280000	-1.961935000
O	-2.756248000	1.378041000	-3.378087000
O	-0.426322000	4.136347000	-1.901550000
O	1.050166000	1.378062000	-4.231527000
O	-3.095964000	-3.665256000	-1.961972000
O	-1.134002000	0.000027000	-5.057915000
O	-2.756237000	-1.377999000	-3.378088000
O	1.050148000	-1.377993000	-4.231511000
O	-0.426360000	-4.136345000	-1.901625000
O	-1.961947000	3.665260000	3.095976000
O	2.756237000	1.377999000	3.378088000
O	0.426360000	4.136345000	1.901625000
O	-1.050148000	1.377993000	4.231511000
O	1.134002000	-0.000027000	5.057915000
O	-1.961963000	-3.665280000	3.095941000
O	2.756248000	-1.378041000	3.378087000
O	-1.050166000	-1.378062000	4.231527000
O	0.426322000	-4.136347000	1.901550000
O	3.095964000	3.665256000	1.961972000
O	1.961963000	3.665280000	-3.095941000
O	4.231496000	1.378001000	1.050152000
O	3.378086000	1.377990000	-2.756252000
O	1.901611000	4.136360000	-0.426322000
O	5.057911000	-0.000007000	-1.134002000
O	4.231491000	-1.378043000	1.050151000
O	3.095944000	-3.665280000	1.961935000
O	1.961947000	-3.665260000	-3.095976000
O	1.901562000	-4.136340000	-0.426344000
O	3.378106000	-1.378013000	-2.756285000
Si	1.854864000	4.519370000	1.175470000

H	1.981858000	5.981658000	1.255953000
Si	-1.854879000	4.519403000	-1.175449000
H	-1.981830000	5.981678000	-1.255896000
H	-1.260327000	6.061225000	1.988839000
Si	1.175470000	4.519386000	-1.854866000
H	1.255971000	5.981658000	-1.981870000
Si	3.817401000	2.195929000	2.419153000
H	5.052561000	2.346267000	3.201893000
H	3.859407000	-0.000033000	5.233309000
Si	4.992854000	-0.000010000	0.564260000
H	6.308518000	-0.000020000	1.219954000
Si	3.817399000	-2.195966000	2.419137000
H	5.052552000	-2.346316000	3.201872000
Si	1.854879000	-4.519403000	1.175449000
H	1.981830000	-5.981678000	1.255896000
Si	-1.175470000	-4.519386000	1.854866000
H	-1.255971000	-5.981658000	1.981870000
H	1.260327000	-6.061225000	-1.988839000
Si	-1.854864000	-4.519370000	-1.175470000
H	-1.981858000	-5.981658000	-1.255953000
Si	-3.817401000	-2.195929000	-2.419153000
H	-5.052561000	-2.346267000	-3.201893000
Si	-4.992854000	0.000010000	-0.564260000
H	-6.308518000	0.000020000	-1.219954000
H	-3.859407000	0.000033000	-5.233309000
Si	-3.817399000	2.195966000	-2.419137000
H	-5.052552000	2.346316000	-3.201872000
Si	-0.564259000	-0.000015000	4.992827000
H	-1.219957000	-0.000027000	6.308491000
H	-3.244465000	-2.354547000	5.119733000
Si	-2.419123000	2.195945000	3.817389000
H	-3.201857000	2.346332000	5.052536000
Si	-4.274010000	-0.000012000	2.641917000
H	-5.183770000	-0.000007000	3.796562000
Si	0.564259000	0.000015000	-4.992827000
H	1.219957000	0.000027000	-6.308491000
H	3.244465000	2.354547000	-5.119733000
Si	2.419123000	-2.195945000	-3.817389000
H	3.201857000	-2.346332000	-5.052536000
Si	4.274010000	0.000012000	-2.641917000
H	5.183770000	0.000007000	-3.796562000
Al	2.641938000	-0.000021000	4.274007000
Al	-2.641938000	0.000021000	-4.274007000
Al	-1.175465000	4.519365000	1.854900000
Al	1.175465000	-4.519365000	-1.854900000
Al	-2.419141000	-2.195982000	3.817356000

Al	2.419141000	2.195982000	-3.817356000
Ag	-2.689327000	2.010015000	0.625060000
Ag	2.714326000	1.974264000	-0.658280000
Ag	0.609691000	-1.979445000	2.812637000
Ag	-0.628029000	-2.018120000	-2.779515000
Ag	0.628029000	2.018120000	2.779515000
Ag	-0.609691000	1.979445000	-2.812637000
Ag	-2.714326000	-1.974264000	0.658280000
Ag	2.689327000	-2.010015000	-0.625060000
Ag	-1.045963000	-0.002593000	1.690229000
Ag	-1.649955000	0.000783000	-1.070699000
Ag	0.003676000	1.962320000	0.002217000
Ag	1.045963000	0.002593000	-1.690229000
Ag	1.649955000	-0.000783000	1.070699000
Ag	-0.003676000	-1.962320000	-0.002217000

$[Ag_{14}(Si_{24}H_{24}O_{36})]^{6+}$:

O	1.378007000	4.136354000	1.378007000
O	1.378007000	1.378007000	4.136354000
O	4.136354000	1.378007000	1.378007000
O	0.000000000	3.665274000	3.665274000
O	-1.378007000	4.136354000	1.378007000
O	-4.136354000	1.378007000	1.378007000
O	-1.378007000	1.378007000	4.136354000
O	3.665274000	3.665274000	0.000000000
O	1.378007000	4.136354000	-1.378007000
O	4.136354000	1.378007000	-1.378007000
O	1.378007000	1.378007000	-4.136354000
O	-3.665274000	3.665274000	0.000000000
O	0.000000000	3.665274000	-3.665274000
O	-1.378007000	4.136354000	-1.378007000
O	-1.378007000	1.378007000	-4.136354000
O	-4.136354000	1.378007000	-1.378007000
O	3.665274000	0.000000000	3.665274000
O	1.378007000	-4.136354000	1.378007000
O	4.136354000	-1.378007000	1.378007000
O	1.378007000	-1.378007000	4.136354000
O	0.000000000	-3.665274000	3.665274000
O	-3.665274000	0.000000000	3.665274000
O	-1.378007000	-4.136354000	1.378007000
O	-1.378007000	-1.378007000	4.136354000
O	-4.136354000	-1.378007000	1.378007000
O	3.665274000	-3.665274000	0.000000000
O	3.665274000	0.000000000	-3.665274000
O	1.378007000	-4.136354000	-1.378007000

O	1.378007000	-1.378007000	-4.136354000
O	4.136354000	-1.378007000	-1.378007000
O	0.000000000	-3.665274000	-3.665274000
O	-1.378007000	-4.136354000	-1.378007000
O	-3.665274000	-3.665274000	0.000000000
O	-3.665274000	0.000000000	-3.665274000
O	-4.136354000	-1.378007000	-1.378007000
O	-1.378007000	-1.378007000	-4.136354000
Si	4.519375000	-2.195954000	0.000000000
H	5.981668000	-2.346285000	0.000000000
Si	4.519375000	0.000000000	2.195954000
H	5.981668000	0.000000000	2.346285000
Si	4.519375000	0.000000000	-2.195954000
H	5.981668000	0.000000000	-2.346285000
Si	4.519375000	2.195954000	0.000000000
H	5.981668000	2.346285000	0.000000000
Si	2.195954000	4.519375000	0.000000000
H	2.346285000	5.981668000	0.000000000
Si	0.000000000	4.519375000	2.195954000
H	0.000000000	5.981668000	2.346285000
Si	0.000000000	4.519375000	-2.195954000
H	0.000000000	5.981668000	-2.346285000
Si	-2.195954000	4.519375000	0.000000000
H	-2.346285000	5.981668000	0.000000000
Si	-4.519375000	2.195954000	0.000000000
H	-5.981668000	2.346285000	0.000000000
Si	-4.519375000	0.000000000	2.195954000
H	-5.981668000	0.000000000	2.346285000
Si	-4.519375000	0.000000000	-2.195954000
H	-5.981668000	0.000000000	-2.346285000
Si	-4.519375000	-2.195954000	0.000000000
H	-5.981668000	-2.346285000	0.000000000
Si	-2.195954000	-4.519375000	0.000000000
H	-2.346285000	-5.981668000	0.000000000
Si	0.000000000	-4.519375000	-2.195954000
H	0.000000000	-5.981668000	-2.346285000
Si	0.000000000	-4.519375000	2.195954000
H	0.000000000	-5.981668000	2.346285000
Si	2.195954000	-4.519375000	0.000000000
H	2.346285000	-5.981668000	0.000000000
Si	0.000000000	-2.195954000	4.519375000
H	0.000000000	-2.346285000	5.981668000
Si	-2.195954000	0.000000000	4.519375000
H	-2.346285000	0.000000000	5.981668000
Si	2.195954000	0.000000000	4.519375000
H	2.346285000	0.000000000	5.981668000

Si	0.000000000	2.195954000	4.519375000
H	0.000000000	2.346285000	5.981668000
Si	0.000000000	-2.195954000	-4.519375000
H	0.000000000	-2.346285000	-5.981668000
Si	-2.195954000	0.000000000	-4.519375000
H	-2.346285000	0.000000000	-5.981668000
Si	2.195954000	0.000000000	-4.519375000
H	2.346285000	0.000000000	-5.981668000
Si	0.000000000	2.195954000	-4.519375000
H	0.000000000	2.346285000	-5.981668000
Ag	2.019181000	2.019181000	2.019181000
Ag	2.019181000	-2.019181000	-2.019181000
Ag	-2.019181000	-2.019181000	2.019181000
Ag	-2.019181000	2.019181000	-2.019181000
Ag	2.019181000	-2.019181000	2.019181000
Ag	2.019181000	2.019181000	-2.019181000
Ag	-2.019181000	2.019181000	2.019181000
Ag	-2.019181000	-2.019181000	-2.019181000
Ag	0.000000000	0.000000000	1.963906000
Ag	0.000000000	1.963906000	0.000000000
Ag	1.963906000	0.000000000	0.000000000
Ag	0.000000000	0.000000000	-1.963906000
Ag	0.000000000	-1.963906000	0.000000000
Ag	-1.963906000	0.000000000	0.000000000

Cartesian Coordinate (in Angstrom) of Ag_8

optimized at B3LYP/LANL2DZ

Ag	-1.665404000	-1.665404000	-1.665404000
Ag	1.665404000	-1.665404000	1.665404000
Ag	-1.665404000	1.665404000	1.665404000
Ag	1.665404000	1.665404000	-1.665404000
Ag	1.038277000	1.038277000	1.038277000
Ag	-1.038277000	-1.038277000	1.038277000
Ag	-1.038277000	1.038277000	-1.038277000
Ag	1.038277000	-1.038277000	-1.038277000

Cartesian Coordinate (in Angstrom) of $[Ag_8(Si_{24}H_{36}O_{24})]$

optimized at B3LYP/LANL2DZ

O	-1.340818000	1.341134000	4.596823000

O	-1.341134000	4.596823000	1.340818000
O	-4.596823000	1.340818000	1.341134000
O	0.008400000	3.470561000	3.470597000
O	1.355233000	1.354864000	4.591903000
O	4.591903000	1.355233000	1.354864000
O	1.354864000	4.591903000	1.355233000
O	-3.470597000	-0.008400000	3.470561000
O	-1.355233000	-1.354864000	4.591903000
O	-4.591903000	-1.355233000	1.354864000
O	-1.354864000	-4.591903000	1.355233000
O	3.470597000	0.008400000	3.470561000
O	-0.008400000	-3.470561000	3.470597000
O	1.340818000	-1.341134000	4.596823000
O	1.341134000	-4.596823000	1.340818000
O	4.596823000	-1.340818000	1.341134000
O	-3.470561000	3.470597000	-0.008400000
O	-1.355233000	1.354864000	-4.591903000
O	-4.591903000	1.355233000	-1.354864000
O	-1.354864000	4.591903000	-1.355233000
O	-0.008400000	3.470561000	-3.470597000
O	3.470561000	3.470597000	0.008400000
O	1.340818000	1.341134000	-4.596823000
O	1.341134000	4.596823000	-1.340818000
O	4.596823000	1.340818000	-1.341134000
O	-3.470597000	0.008400000	-3.470561000
O	-3.470561000	-3.470597000	0.008400000
O	-1.340818000	-1.341134000	-4.596823000
O	-1.341134000	-4.596823000	-1.340818000
O	-4.596823000	-1.340818000	-1.341134000
O	0.008400000	-3.470561000	-3.470597000
O	1.355233000	-1.354864000	-4.591903000
O	3.470597000	-0.008400000	-3.470561000
O	3.470561000	-3.470597000	-0.008400000
O	4.591903000	-1.355233000	-1.354864000
O	1.354864000	-4.591903000	-1.355233000
Si	4.663018000	-2.321972000	0.002730000
H	5.955332000	-3.029758000	0.005702000
Si	4.663018000	2.321972000	-0.002730000
H	5.955332000	3.029758000	-0.005702000
Si	0.002730000	-4.663018000	2.321972000
H	0.005702000	-5.955332000	3.029758000
Si	2.321972000	-0.002730000	4.663018000
H	3.029758000	-0.005702000	5.955332000
Si	-0.002730000	4.663018000	2.321972000
H	-0.005702000	5.955332000	3.029758000
Si	0.002730000	4.663018000	-2.321972000
H	0.005702000	5.955332000	-3.029758000
Si	-4.663018000	2.321972000	0.002730000
H	-5.955332000	3.029758000	0.005702000
Si	-4.663018000	-2.321972000	-0.002730000
H	-5.955332000	-3.029758000	-0.005702000

Si	-2.321972000	-0.002730000	-4.663018000
H	-3.029758000	-0.005702000	-5.955332000
Si	-2.321972000	0.002730000	4.663018000
H	-3.029758000	0.005702000	5.955332000
Si	-0.002730000	-4.663018000	-2.321972000
H	-0.005702000	-5.955332000	-3.029758000
Si	2.321972000	0.002730000	-4.663018000
H	3.029758000	0.005702000	-5.955332000
Ag	1.624783000	-1.624783000	-1.624783000
Ag	1.624783000	1.624783000	1.624783000
Ag	-1.624783000	-1.624783000	1.624783000
Ag	-1.624783000	1.624783000	-1.624783000
Ag	-1.024879000	1.024879000	1.024879000
Ag	1.024879000	-1.024879000	1.024879000
Ag	-1.024879000	-1.024879000	-1.024879000
Ag	1.024879000	1.024879000	-1.024879000
Si	-4.662987000	-0.002035000	-2.321948000
H	-5.955428000	-0.004403000	-3.029520000
Si	0.002035000	2.321948000	-4.662987000
H	0.004403000	3.029520000	-5.955428000
Si	-2.321948000	4.662987000	0.002035000
H	-3.029520000	5.955428000	0.004403000
Si	-4.662987000	0.002035000	2.321948000
H	-5.955428000	0.004403000	3.029520000
Si	-2.321948000	-4.662987000	-0.002035000
H	-3.029520000	-5.955428000	-0.004403000
Si	0.002035000	-2.321948000	4.662987000
H	0.004403000	-3.029520000	5.955428000
Si	-0.002035000	2.321948000	4.662987000
H	-0.004403000	3.029520000	5.955428000
Si	2.321948000	-4.662987000	0.002035000
H	3.029520000	-5.955428000	0.004403000
Si	4.662987000	-0.002035000	2.321948000
H	5.955428000	-0.004403000	3.029520000
Si	2.321948000	4.662987000	-0.002035000
H	3.029520000	5.955428000	-0.004403000
Si	-0.002035000	-2.321948000	-4.662987000
H	-0.004403000	-3.029520000	-5.955428000
Si	4.662987000	0.002035000	-2.321948000
H	5.955428000	0.004403000	-3.029520000