Electronic Supplementary Information for:

Shapeshifting: Ligation by 1,4-cyclohexadiene induces a structural change in Ag5+

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Table S1. Sequential gas-phase binding enthalpies of ethene to Ag_3^+ at 0 K obtained from experiments (Exp.) and theory.

	0 K ΔH_n, eV		
		Theory	
n	**Exp. MKB[a,b]**	**MKB[b]**	**This Work[c]**
1	0.93	0.72	0.84
2	0.85	0.61	0.73
3	0.74	0.48	0.59
4	0.24	--	--

[a] Manard, M. J.; Kemper, P. R.; Bowers, M. T. *J. Am. Chem. Soc.* **2005**, *127*, 9994-9995. [b] Manard, M. J.; Kemper, P. R.; Bowers, M. T. *Int. J. Mass Spectrom.* **2006**, *249-250*, 252-262: Calculated using the B3LYP hybrid functional with the 6-31+G** basis set for carbon and hydrogen, and a valence double-zeta basis set and a (5s6p4d)→[3s3p2d] contraction of the Hay-Wadt (n + 1) effective core potential for silver. [c] Calculated using computational method described in main text.

Table S2. Sequential gas-phase binding enthalpies of ethene to Ag_5^+ at 0 and 298 K obtained from experiments (Exp.) and theory.

	298 K ΔH_n, kJ/mol			0 K ΔH_n, kJ/mol		
		Theory			Theory	
n	**Exp. MKB[a,b]**	**MKB[b]**	**This Work[c]**	**Exp. MKB[a,b]**	**MKB[b]**	**This Work[c]**
1	78.7	58.1	62.9	78.2	53.3	64.4
2	77.0	51.2	58.9	76.1	46.3	55.6
3	108.4	45.1	56.4	105.4	37.4	58.6
4	38.9	18.3	23.0	37.2	15.0	23.8
5	28.9	11.3	15.5	28.0	8.7	10.9
6	18.8	--	--	18.8	--	--

[a] Manard, M. J.; Kemper, P. R.; Bowers, M. T. *J. Am. Chem. Soc.* **2005**, *127*, 9994-9995. [b] Manard, M. J.; Kemper, P. R.; Bowers, M. T. *Int. J. Mass Spectrom.* **2006**, *249-250*, 252-262: Calculated using the B3LYP hybrid functional with the 6-31+G** basis set for carbon and hydrogen, and a valence double-zeta basis set and a (5s6p4d)→[3s3p2d] contraction of the Hay-Wadt (n + 1) effective core potential for silver. [c] Calculated using computational method described in main text.

Cartesian Coordinates of Optimized Molecular Geometries. 0 K enthalpy values are in Hartrees and *x,y,z* coordinate values are in Angstroms.

Ag_3^+ Global Minimum Structure (Figure 2, top left)
0 K Enthalpy: -440.841631

Ag	1.36581784	-0.78855530	-0.00000000
Ag	-0.00000000	1.57711060	-0.00000000
Ag	-1.36581784	-0.78855530	-0.00000000

Ag_3^+(cH) Global Minimum Structure (Figure 2, top right)
0 K Enthalpy: -675.447167

Ag	-2.24690000	-1.03593800	0.04121200
Ag	0.43919900	-0.40590200	-0.11066700
Ag	-1.52333800	1.53189000	0.02347000
C	2.67148200	-1.32240700	0.41299200
C	3.33337800	-0.50318400	1.49126100
C	2.70335500	-0.97557700	-0.90541600
H	2.29223900	-2.30503600	0.68899200
C	3.68998800	0.91036700	1.01342700
H	4.24216400	-1.04117200	1.79407300
H	2.70583900	-0.47523000	2.38770500
C	3.43995800	0.23920700	-1.42654100
H	2.32959400	-1.68527000	-1.64168100
C	4.35887800	0.86860800	-0.36615800
H	4.34411600	1.39353200	1.74229100
H	2.77894500	1.52293300	0.96389700
H	4.02142100	-0.07233900	-2.30046600
H	2.72714000	0.97881900	-1.81257400
H	4.65598800	1.87075600	-0.68236900
H	5.27912200	0.27859300	-0.29594500

$Ag_3^+(cH)_2$ Global Minimum Structure (Figure 2, lower)
0 K Enthalpy: -910.04593

Ag	1.41399900	-0.15379900	-0.24582800
Ag	-1.38475700	-0.21872900	-0.06614900
Ag	-0.01569400	2.08606800	0.19059100
C	-3.33513200	-1.54232300	-0.84864100
C	-4.36977500	-0.62637200	-1.45187300
C	-3.24019500	-1.77313500	0.48921500
H	-2.74418900	-2.14988800	-1.53173100
C	-5.03227900	0.27818500	-0.40422300
H	-5.12436900	-1.26167400	-1.93560100
H	-3.92823600	-0.03743700	-2.26214600

C	-4.18449200	-1.16866200	1.50525300
H	-2.56010300	-2.54733500	0.84005500
C	-5.41448900	-0.52163200	0.84734400
H	-5.91313300	0.75926500	-0.83518900
H	-4.34324000	1.08727200	-0.12736600
H	-4.49235300	-1.96223100	2.19394300
H	-3.65123900	-0.44104600	2.12991100
H	-5.92839300	0.11556900	1.57042900
H	-6.12353100	-1.30757700	0.56464300
C	3.20050100	-1.86698300	-0.02488000
C	3.90939000	-1.69926700	1.29533200
C	3.51451800	-1.13969400	-1.13156300
H	2.51620700	-2.70769800	-0.12479500
C	4.72102300	-0.39883600	1.35978800
H	4.57193000	-2.56626300	1.42299300
H	3.19343900	-1.76006600	2.12121800
C	4.63058000	-0.11859600	-1.16504700
H	3.05474800	-1.40605800	-2.08153100
C	5.53521700	-0.19826700	0.07553500
H	5.37893400	-0.41588300	2.23152500
H	4.04073200	0.45156300	1.50231900
H	5.21435100	-0.28796700	-2.07581900
H	4.21572900	0.89103300	-1.27867200
H	6.14886700	0.70266100	0.14420000
H	6.22788900	-1.03911000	-0.04067800

Ag_3^+(1,4-cHD) Global Minimum Structure (Figure 3, upper panel, bidentate structure)
0 K Enthalpy: -674.243654

H	2.53162600	-2.20301000	-1.21330700
C	2.51057600	-1.25874100	-0.67567500
C	2.66036100	0.00021600	-1.49305500
C	2.51012300	-1.25880100	0.67616800
C	2.51030000	1.25911300	-0.67556800
H	3.65977500	0.00034900	-1.95319700
H	1.96897000	0.00014600	-2.34292100
C	2.65937900	0.00008400	1.49380000
H	2.53086100	-2.20312900	1.21371000
C	2.50989500	1.25902900	0.67634500
H	2.53112300	2.20341500	-1.21315000
H	3.65848000	0.00015600	1.95462400
H	1.96741800	-0.00002900	2.34320400
H	2.53042300	2.20328500	1.21402400
Ag	-2.37025900	-0.00009300	0.00018300
Ag	-0.02260000	-1.37017200	-0.00024900
Ag	-0.02293900	1.37012500	-0.00025400

Ag_3^+(1,4-cHD) Lowest Energy Monodentate Structure (Figure 3, upper right structure)
0 K Enthalpy: -674.241521

H	2.48848000	-2.12337900	-1.21499000
C	2.77964200	-1.22240100	-0.68030700
C	3.36747600	-0.08994900	-1.48281400
C	2.77954500	-1.22250400	0.68016600
C	3.52394100	1.16861900	-0.66718300
H	4.34944200	-0.41660500	-1.85876500
H	2.77543300	0.09399500	-2.38539800
C	3.36731100	-0.09018300	1.48291300
H	2.48834100	-2.12357300	1.21468000
C	3.52385800	1.16851700	0.66749100
H	3.67653300	2.09462100	-1.21153300
H	4.34925200	-0.41689900	1.85887900
H	2.77519300	0.09361500	2.38547500
H	3.67637800	2.09444000	1.21199600
Ag	-1.37448000	1.53163100	-0.00000100
Ag	0.52375900	-0.46903400	-0.00006700
Ag	-2.18395300	-1.01087000	0.00002700

Ag_3^+(1,4-cHD)$_2$ Global Minimum Structure (Figure 3, middle panel)
0 K Enthalpy: -907.633742

H	-2.70121700	-2.60639400	0.91186400
C	-3.30107900	-1.78256700	0.53240600
C	-4.15115700	-1.02764800	1.52185400
C	-3.39695900	-1.59037400	-0.80859100
C	-4.81880800	0.17668100	0.90933500
H	-4.91221200	-1.71977200	1.91369300
H	-3.56048200	-0.74398500	2.40012100
C	-4.36326300	-0.60758000	-1.41862500
H	-2.87167500	-2.26226900	-1.48321000
C	-4.91375000	0.36487400	-0.40730500
H	-5.25709800	0.89625000	1.59298400
H	-5.18542700	-1.17964300	-1.87530100
H	-3.89794400	-0.07935000	-2.25830900
H	-5.42950000	1.23742800	-0.79446100
Ag	-0.00003400	2.00163700	0.04979600
Ag	-1.40159200	-0.29325500	-0.07564300
Ag	1.40151700	-0.29320600	-0.07530400
H	2.70187800	-2.60666500	0.91191500
C	3.30157000	-1.78277700	0.53234000
C	4.15187900	-1.02782700	1.52160200
C	3.39691600	-1.59037700	-0.80861800
C	4.81902700	0.17675600	0.90901300

H	3.56145900	-0.74438100	2.40011000
H	4.91321600	-1.71985500	1.91305300
C	4.36287700	-0.60735000	-1.41889400
H	2.87144800	-2.26224200	-1.48311500
C	4.91345300	0.36514300	-0.40764900
H	5.25736500	0.89635100	1.59259800
H	3.89720200	-0.07912700	-2.25838000
H	5.18501800	-1.17922900	-1.87582900
H	5.42884600	1.23787400	-0.79487400

Ag_3^+(1,4-cHD)$_2$ Lowest Energy Bidentate Structure (Figure 3, lower panel)
0 K Enthalpy: -907.629843

H	3.97420100	-1.76220100	-1.18037800
C	3.78406500	-0.83409100	-0.64813400
C	3.68906300	0.42300800	-1.47538700
C	3.76811600	-0.83012300	0.69923600
C	3.33770500	1.64201000	-0.66045900
H	4.65613600	0.59490600	-1.97028000
H	2.97945800	0.29080000	-2.30105300
C	3.65383700	0.43166900	1.51676600
H	3.94556500	-1.75510400	1.24122400
C	3.32214400	1.64602000	0.68687700
H	3.19298200	2.57292400	-1.20205400
H	4.60885800	0.60619800	2.03363900
H	2.92460900	0.30417500	2.32593700
H	3.16504700	2.58012800	1.21944600
Ag	-1.39703200	-0.48360500	-0.01774400
Ag	1.19986700	-1.37761000	-0.00245000
Ag	0.72174600	1.26214200	-0.01376000
H	-4.55131600	2.42229900	-1.12441500
C	-4.41249500	1.47574600	-0.61205100
C	-4.27105400	0.24809100	-1.47425700
C	-4.40581200	1.43569200	0.72066600
C	-3.79277000	-0.95197300	-0.69833700
H	-5.24049900	-0.00268700	-1.93100100
H	-3.60993800	0.44323400	-2.32671100
C	-4.25663800	0.15872600	1.50652400
H	-4.53911400	2.34983300	1.29016100
C	-3.78650500	-0.99269100	0.65558500
H	-3.57107300	-1.85586100	-1.26063200
H	-5.22168000	-0.11885000	1.95699000
H	-3.58680200	0.30274300	2.36229500
H	-3.55969100	-1.92859800	1.16053700

Ag_5^+ Twisted Bowtie Structure (Figure 4, structure a)
0 K Enthalpy: -734.93893

Ag	2.45823100	0.94732900	0.93403400
Ag	2.45979200	-0.94668400	-0.93343100
Ag	0.00010300	-0.00079500	-0.00050700
Ag	-2.45892500	0.93788300	-0.94293900
Ag	-2.45920100	-0.93773400	0.94284300

Ag_5^+ Planar Bowtie Structure (Figure 4, structure b)
0 K Enthalpy: -734.938146

Ag	-1.32813100	2.46231500	0.00000000
Ag	1.32813900	2.46239400	0.00000000
Ag	-0.00001500	-0.00000100	0.00000000
Ag	-1.32813100	-2.46241600	0.00000000
Ag	1.32813900	-2.46229200	0.00000000

Ag_5^+ Capped Tetrahedral Structure (Figure 4, structure c)
0 K Enthalpy: -734.915275

Ag	1.68592900	-1.00156200	0.98988500
Ag	-0.32390100	0.98996200	1.01038600
Ag	-0.32363600	-0.99929800	-1.00152400
Ag	1.66772600	1.01087600	-0.99877100
Ag	-2.70611800	0.00002300	0.00002300

Ag_5^+ Trigonal Bipyramidal Structure (Figure 4, structure d)
0 K Enthalpy: -734.912812

Ag	-0.04093800	-0.71329000	1.41563300
Ag	-0.00510200	1.58280600	-0.09231200
Ag	0.04698700	-0.87153500	-1.32600500
Ag	-2.40153600	-0.00311900	-0.02360300
Ag	2.40058900	0.00513800	0.02628700

Ag_5^+(1,4-cHD) Global Minimum Structure (Figure 5, structure a)
0 K Enthalpy: -968.340659

H	2.19997500	3.28306200	-1.21406500
C	1.25674800	3.22739600	-0.67693700
C	-0.00235900	3.35978400	-1.49497800
C	1.25701100	3.22694800	0.67684700
C	-1.26103400	3.22629400	-0.67634100
H	-0.00284000	4.35408900	-1.96649100
H	-0.00226900	2.65903900	-2.33627800

C	-0.00174100	3.35866200	1.49554300
H	2.20043000	3.28228100	1.21367000
C	-1.26073600	3.22574900	0.67743800
H	-2.20453800	3.28097800	-1.21307400
H	-0.00212800	4.35258600	1.96784800
H	-0.00122300	2.65725400	2.33629900
H	-2.20395200	3.28008900	1.21472300
Ag	-2.74060000	-1.64840600	-0.00035200
Ag	0.00085300	-1.41546900	0.00052500
Ag	1.67818300	0.81406700	-0.00042600
Ag	-1.67900200	0.81240400	0.00005200
Ag	2.74246300	-1.64553900	-0.00005500

Ag_5^+(1,4-cHD) Lowest Energy Monodentate Structure (Figure 5, structure b)
0 K Enthalpy: -968.329598

Ag	3.14808500	-0.55710600	-1.32375500
Ag	3.13172100	-0.60475200	1.32470700
Ag	0.85610800	0.36706100	0.00369500
Ag	-1.91209400	-0.21192400	-0.05688200
Ag	-1.03664400	2.32185800	0.04796100
H	-2.57886400	-2.78239100	0.91746900
C	-3.36953600	-2.15344800	0.51521600
C	-4.42059300	-1.65896700	1.47528600
C	-3.47475800	-1.99435900	-0.82900000
C	-5.38189200	-0.69194400	0.83344500
H	-4.96821100	-2.53317200	1.85943400
H	-3.95420300	-1.21620100	2.36265000
C	-4.65175800	-1.30993500	-1.47504700
H	-2.76681100	-2.49811400	-1.48285100
C	-5.48537000	-0.53588100	-0.48655200
H	-6.02542400	-0.12536300	1.49833600
H	-5.26741000	-2.08118200	-1.96267800
H	-4.31957000	-0.66516200	-2.29661900
H	-6.21334500	0.15734800	-0.89488400

Ag_5^+(1,4-cHD) Higher Energy Local Minimum Bidentate Structure (Figure 5, structure c)
0 K Enthalpy: -968.324061

Ag	-3.30038200	-0.95199900	-0.90323300
Ag	-3.28258900	0.96258400	0.91185900
Ag	-0.78620000	-0.00751200	-0.00694700
Ag	1.64332700	0.93682200	-0.95380100
Ag	1.64247300	-0.94707700	0.94770300
H	4.31394600	2.41497800	-0.71434800
C	4.30349400	1.36948700	-0.41826500

C	4.42056700	1.07375400	1.05512300
C	4.30758100	0.41019200	-1.36350700
C	4.30617700	-0.39509800	1.37279400
H	5.39416300	1.43902200	1.41350700
H	3.68370000	1.65196900	1.62588100
C	4.42894800	-1.05809700	-1.04550100
H	4.32143900	0.69073100	-2.41323900
C	4.31017000	-1.35436300	0.42766300
H	4.31796600	-0.67545700	2.42257600
H	5.40415500	-1.41964100	-1.40316500
H	3.69528100	-1.63951700	-1.61725700
H	4.32615500	-2.39980500	0.72392900

Ag_5^+(1,4-cHD) Higher Energy Local Minimum Bidentate Structure (Figure 5, structure d)
0 K Enthalpy: -968.316875

Ag	1.41522400	-0.67071100	1.06322500
Ag	-0.05511500	0.68368500	-0.93696500
Ag	-1.39941200	-0.93695700	0.95151400
Ag	0.21620400	-2.12985300	-1.04352700
Ag	-2.57294900	1.37948800	-0.01419600
H	2.87870000	1.50879500	2.45899500
C	2.72914100	1.59520100	1.38616500
C	1.85753000	2.72673300	0.89858800
C	3.44523600	0.81604300	0.54335800
C	1.55512200	2.64595400	-0.57817700
H	0.93644100	2.79650700	1.48378800
H	2.38549500	3.67301000	1.09306200
C	3.41342000	1.00039900	-0.95258400
H	4.17208500	0.11383400	0.94313400
C	2.25366800	1.84638600	-1.41868400
H	0.84481200	3.36342600	-0.97727700
H	3.43010700	0.03504400	-1.46632700
H	4.34708200	1.49726400	-1.25883600
H	2.09479200	1.92221400	-2.49092400

Ag_5^+(1,4-cHD) Higher Energy Local Minimum Bidentate Structure (Figure 5, structure e)
0 K Enthalpy: -968.314948

H	2.19997500	3.28306200	-1.21406500
C	1.25674800	3.22739600	-0.67693700
C	-0.00235900	3.35978400	-1.49497800
C	1.25701100	3.22694800	0.67684700
C	-1.26103400	3.22629400	-0.67634100
H	-0.00284000	4.35408900	-1.96649100
H	-0.00226900	2.65903900	-2.33627800

C	-0.00174100	3.35866200	1.49554300
H	2.20043000	3.28228100	1.21367000
C	-1.26073600	3.22574900	0.67743800
H	-2.20453800	3.28097800	-1.21307400
H	-0.00212800	4.35258600	1.96784800
H	-0.00122300	2.65725400	2.33629900
H	-2.20395200	3.28008900	1.21472300
Ag	-2.74060000	-1.64840600	-0.00035200
Ag	0.00085300	-1.41546900	0.00052500
Ag	1.67818300	0.81406700	-0.00042600
Ag	-1.67900200	0.81240400	0.00005200
Ag	2.74246300	-1.64553900	-0.00005500

Ag_5^+(cH) Global Minimum Structure (Figure 5, bottom panel)
0 K Enthalpy: -969.535741

Ag	3.12505700	-0.77783400	-1.30726200
Ag	3.20242900	-0.53235600	1.32904700
Ag	0.91854000	0.38012200	-0.02007800
Ag	-1.86352700	-0.09837100	0.15185900
Ag	-0.91044600	2.39014800	-0.16704200
H	-4.82372400	0.18808800	-1.11771000
C	-5.28358000	-0.80783600	-1.06850300
C	-4.22430000	-1.87767200	-1.36634400
C	-5.90117100	-1.02074900	0.31910500
H	-6.05672300	-0.82828100	-1.83979400
C	-3.29524500	-2.10616900	-0.20069000
H	-4.70840700	-2.83788300	-1.59128300
H	-3.65081900	-1.62698800	-2.26460500
C	-4.84074400	-0.94398500	1.42974100
H	-6.68834600	-0.28730900	0.50748700
H	-6.37886700	-2.00631500	0.34869000
C	-3.56632800	-1.66994700	1.05905700
H	-2.45009500	-2.77438800	-0.35600400
H	-4.61999900	0.10068900	1.68280400
H	-5.22437300	-1.38507600	2.35560900
H	-2.91692600	-1.98473300	1.87399900

Ag_7^+ (Figure 6)
0 K Enthalpy: -1029.048402

Ag	0.88882800	2.62839500	-0.19300800
Ag	-1.83213300	2.08159100	0.20079400
Ag	0.00074500	0.00033900	-0.00015500
Ag	2.72151900	0.54268500	0.19165600

Ag	-2.71935700	-0.54343300	-0.20689400
Ag	1.83079600	-2.08384700	-0.19771000
Ag	-0.89039800	-2.62572900	0.20531800

Ag_9^+ (Figure 6)
0 K Enthalpy: -1323.153678

Ag	0.15327900	-1.62339200	-1.48780000
Ag	-1.48300300	0.68082400	-1.48747300
Ag	1.33069300	0.94511200	-1.48704800
Ag	0.15234300	-1.62508400	1.48679600
Ag	-1.48357400	0.67970500	1.48840600
Ag	1.33012600	0.94352400	1.48794900
Ag	-2.28443000	-1.62124200	-0.00141400
Ag	2.54606800	-1.16757000	0.00012400
Ag	-0.26150300	2.78812300	0.00046000

Ag_7^+(1,4,5,8-tetrahydronaphthalene) (Figure 6)
0 K Enthalpy: -1417.220683

C	-0.00068600	3.17980700	0.67933500
C	1.27947100	3.28503400	1.48337500
C	-0.00022200	3.18089300	-0.67756800
C	2.53826500	3.11989100	0.67607200
H	1.30819500	4.27837700	1.95787400
H	1.26434500	2.58153300	2.32349100
C	1.28045700	3.28758100	-1.48063300
C	2.53871000	3.12104100	-0.67276700
H	3.47884300	3.13675000	1.22008700
H	1.30948500	4.28178000	-1.95332200
H	1.26594700	2.58560100	-2.32203300
H	3.47965600	3.13874900	-1.21611300
Ag	4.24220600	-1.74107900	0.00166900
Ag	1.43799900	-1.67258300	-0.00157400
Ag	0.00004300	0.62076800	-0.00234700
Ag	3.01718700	0.63644500	0.00041900
Ag	-1.43785400	-1.67270000	-0.00180300
C	-2.53919800	3.12033800	-0.67436200
H	-3.47979600	3.13785000	-1.21831300
C	-1.28045200	3.28700900	-1.48145400
H	-1.30952200	4.28106800	-1.95443500
H	-1.26519300	2.58481400	-2.32265500
C	-1.28136000	3.28467500	1.48261900
H	-1.31060200	4.27795600	1.95720600
H	-1.26661900	2.58108600	2.32266600
Ag	-4.24182200	-1.74144300	0.00240400

Ag	-3.01704300	0.63621900	-0.00019500
C	-2.53962300	3.11934500	0.67449200
H	-3.48056200	3.13630000	1.21788800

Ag_9^+(1,4,5,8,9,10-hexahydroanthracene) (Figure 6)
0 K Enthalpy: -1866.092955

C	-1.28138300	3.09986900	0.67638800
C	0.00023500	3.19706000	1.47279000
C	-1.28152500	3.10015000	-0.67560500
C	1.28169000	3.09965200	0.67609500
H	0.00040400	4.16743300	1.99482700
H	0.00029100	2.45538700	2.28137800
C	-0.00008100	3.19764000	-1.47224600
C	1.28154900	3.09990800	-0.67586600
H	-0.00001800	4.16821600	-1.99390500
H	-0.00022400	2.45627900	-2.28111900
Ag	2.96870000	-1.78625700	-0.00016500
Ag	0.00011100	-1.85254300	-0.00050100
Ag	-1.45035200	0.44943400	0.00003000
Ag	1.44964200	0.44833400	-0.00053300
Ag	-2.96825700	-1.78553800	-0.00008200
C	-3.82009300	3.08276100	-0.67300300
H	-4.76071500	3.12076200	-1.21582400
C	-2.55888100	3.20644100	-1.48395500
H	-2.57108000	4.18621600	-1.98632400
H	-2.55655800	2.47889100	-2.30412900
C	-2.55856700	3.20581600	1.48505600
H	-2.57066400	4.18537400	1.98785100
H	-2.55606100	2.47791400	2.30491700
Ag	-5.80777300	-1.68887000	0.00005600
Ag	-4.40966000	0.58908700	0.00020000
C	-3.81994800	3.08247500	0.67431900
H	-4.76045600	3.12024100	1.21735600
C	3.82024600	3.08197900	0.67352900
H	4.76088600	3.11974400	1.21633100
C	3.82010500	3.08220700	-0.67382100
H	4.76063600	3.12016700	-1.21680300
Ag	4.40883600	0.58917200	-0.00070400
Ag	5.80858000	-1.68766000	0.00113000
C	2.55872000	3.20599000	-1.48451400
H	2.57093600	4.18576400	-1.98688600
H	2.55613500	2.47843200	-2.30467300
C	2.55903200	3.20541700	1.48452100
H	2.57133600	4.18497800	1.98730500
H	2.55663100	2.47751200	2.30437400