Cluster of Clusters: A Modular Approach to Large Metal Clusters. Structural Characterization of a 38-Atom Cluster $[(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}]$ Based on Vertex-Sharing Triicosahedra

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Abstract: The crystal and molecular structure of a 38-atom metal cluster, $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$ (**1**), has been determined by single-crystal X-ray crystallography. The cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}\cdot 42EtOH$ crystallizes in a triclinic unit cell of *P*-1 space group with lattice parameters $a = 23.094$ (11) Å, $b = 31.950$ (17) Å, $c = 34.178$ (17) Å, $\alpha = 112.76$ (4)°, $\beta = 90.04$ (3)°, $\gamma = 97.92$ (3)°, and $Z = 2$. The structure was refined to $R_1 = 10.1\%$, $R_2 = 11.8\%$ for 8150 independent reflections with $I > 3\sigma(I)$. The metal framework of **1** can be described as three 13-atom centered icosahedra sharing three vertices in a triangular array plus two capping Ag atoms on the pseudo-3-fold axis. As such, it belongs to a novel series of high-nuclearity Au–Ag clusters whose structures are based on vertex-sharing (centered) icosahedra. Empirical structural rules for these Au–Ag supraclusters are developed. The structural systematics of this new class of supraclusters led to the concept of "cluster of clusters", which is useful in the design, preparation, and characterization of large metal clusters of increasingly high nuclearity via vertex-, edge-, and face-sharing and/or close packing of smaller cluster units as building blocks (viz., a modular approach to large clusters). Simple electron counting of this and related clusters based on a cluster of clusters (C^2) model is also discussed in order to rationalize the observed structural parameters and the electronic requirements.

(I) Introduction

Generally speaking, there are two broad categories of highly symmetrical high-nuclearity metal clusters: the ν_n polyhedral clusters and the s_n supraclusters. A ν_n polyhedral cluster is defined as a cluster with $(n + 1)$ atoms on each edge of the polyhedron.[1] Chart I portrays the early members of the ν_n icosahedral clusters (Mackay[2a] sequence). The magic numbers, defined as the nuclearity (number of atoms) of a cluster, are given in parentheses. These magic numbers represent structurally stable, often closed-shell, configurations of atoms in a cluster and can be observed experimentally. For example, adiabatic jet expansion of inert gas (e.g., Xe) produces van der Waals clusters following the sequence of magic numbers[2b] 1, 13, 55, 147, ...

An s_n supracluster is defined as a cluster of n smaller cluster units fused together via vertex-, edge- or face-sharing.[3,4a] Chart II illustrates the early members of supraclusters based on vertex-sharing centered icosahedral cluster units of 13 atoms. Since these supraclusters, s_n, are made up of smaller cluster units, they are referred to as a *cluster of clusters*.[3,4]

Gold cluster chemistry dates back to the early 1970s with the report of the reduction of $(Ph_3P)AuI$ by $NaBH_4$ to produce $(Ph_3P)_7Au_{11}I_3$.[5] Recent developments[6] in gold phosphine chemistry have produced a novel series of gold clusters up to Au_{13}, which has a centered icosahedral structure [see $\nu_1(13)$ of Chart I].[1] Most, but not all, of the structures of the Au_n ($n < 13$) clusters can be considered as based on this centered icosahedral structure with

Chart I. ν_n Polyhedral Clusters

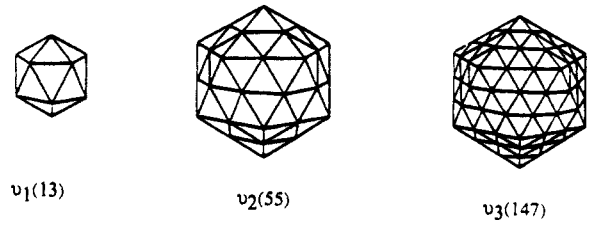
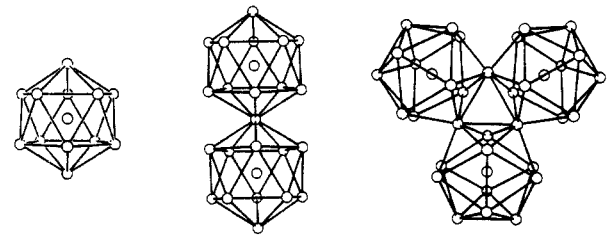


Chart II. s_n Supraclusters: (a) $s_1(13)$ (b) $s_2(25)$ (c) $s_3(36)$



$(13 - n)$ missing vertices. In contrast, similar reactions with the silver analogues produced only insoluble materials.[7]

It occurred to us in 1984 that a combination of Au and Ag might be a fruitful way to produce large metal alloy clusters. This idea resulted in the isolation and structural characterization a 25-atom cluster.[8] Our recent work gives rise to a number of new clusters including a new 25-atom $[(p\text{-Tol}_3P)_{10}Au_{13}Ag_{12}Br_8](PF_6)$,[9] a 37-atom cluster $[(p\text{-Tol}_3P)_{12}Au_{18}Ag_{19}Br_{11}](AsF_6)$,[3a] and the title compound, the 38-atom cluster $[(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}]$. It turns out that the 25-, 37-, and 38-atom clusters follow (or are based on) the magic numbers of the supracluster sequence s_n depicted in Chart II. In other words, the 25 $(Au_{13}Ag_{12})$, 37 $(Au_{18}Ag_{19})$, and 38 $(Au_{18}Ag_{20})$ metal atoms clusters can all be considered as being built from 13-atom centered icosahedral cluster units. Thus, the 25-atom cluster can be described as two ico-

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0002-7863/90/1512-8552$02.50/0

Table I. Summary of Crystal Data, Collection and Reduction of X-ray Data, and Solution and Refinement of Structure of $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}\cdot 42EtOH$ (**1**)

A. Crystal Data	
formula	$(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}\cdot 42EtOH$
crystal color	dark red
crystal shape	prism
crystal size, mm^3	0.1 × 0.1 × 0.05
cell parameters (errors)	
a, Å	23.094 (11)
b, Å	31.950 (17)
c, Å	34.178 (17)
α, deg	112.76 (4)
β, deg	90.04 (3)
γ, deg	97.92 (3)
cell volume, $Å^3$	22992.3 (7)
Z	2
Laue symmetry	triclinic
space group	$P\bar{1}$
systematic absences	no conditions
equivalent positions	$-x, -y, -z$
B. Collection and Reduction of X-ray Diffraction Data	
diffractometer	Enraf-Nonius CAD4
radiation	Mo Kα
wavelength, Å	0.7107
temperature, °C	23 ± 2
scan technique	$\omega/2\theta$
scan rate (limits), deg/min	4–16
scan range, deg	(0.6 + 0.35 tan θ)
no./freq of std reflcns	3/200
2θ limits, deg	$2 < 2\theta < 46$
cutoff of obsd data	$3\sigma(I)$
no. of unique data[a]	64687
octants	$\pm h, \pm k, +l$
linear absorptn coeff, cm^{-1}	68.8
range of transmission	81.46–99.84%
C. Solution and Refinement	
technique of solution	direct method
method of refinement	full-matrix least-squares[b]
std dev	full variance–covariance
isotropic convergence[c]	R_1 = 13.8%, R_2 = 15.2%
isotropic–anisotropic convergence	R_1 = 10.1%, R_2 = 11.8%
max shifts (Δ/σ)	1
data/parameters	8150/581
max resid intens of final diff map, c/Å^3	0.98

[a] The raw intensity is given as $I_{raw} = (20.116 \times ATN)(C - RB)/NPI$, here C is total counts, R is the ratio of scan time to background counting time, B is total background counts, NPI is the ratio of fastest possible scan rate to scan rate for the measurement, and ATN is the attenuator factor (10.7 for Mo in our case). And the observed structure factor amplitude is obtained as the square root of the intensity after correction for Lorentz–polarization: $F_o = (I_{raw}/Lp)^{1/2}$. [b] All lease-squares refinements were based on the minimization of $\sum w_i||F_o| - |F_c||^2$ with the individual weights $w_i = 1/\sigma(F_o)^2$. Atomic scattering factors used for all atoms are from Cromer, D. T.; Waber, J. T. *International Tables for X-ray Crystallography*; Thekynoch Press: Birmingham, England, 1974; Vol. IV, Table 2.2B; Cromer, D. T.; Mann, J. B. X-ray Scattering Factors Computed from Numerical Hartree–Fock Wave Functions. *Acta Crystallogr.* **1968**, *A24*, 321–324. [c] $R_1 = [\sum||F_o| - |F_c||/\sum|F_o|] \times 100\%$ and $R_2 = [\sum w_i||F_o| - |F_c||^2/\sum w_i|F_o|^2]^{1/2} \times 100\%$. See supplementary material for a listing of observed and calculated structure factors.

sahedra sharing a vertex, the 37- and 38-atom clusters as three icosahedra sharing three vertices in a cyclic manner plus one and two capping atoms, respectively.[3,4]

This paper describes the full single-crystal X-ray structure of the 38-atom cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$ (**1**). A communication of this cluster, based on preliminary data, has already appeared.[3b]

It is hoped that the structures of this and related clusters, along with the cluster of clusters (C^2) electron counting approach recently developed by us,[4] will provide new insights in the design and synthesis of very large metal cluster systems via agglomeration of smaller cluster units. We refer to this modular (or building block) approach to large clusters as the "cluster of clusters" approach (cf. Chart II), which is to be contrasted with the "layer by layer" growth of the v_n polyhedral clusters[10-14] (cf. Chart I).

(II) Experiments and Solutions

A. Preparation and Crystallization of Compound 1. To a mixture of $(p\text{-Tol})_3PAuCl$ (0.1 mmol) and $[(p\text{-Tol})_3PAgCl]_4$ (0.025 mmol) in 100 mL of ethanol was added a solution of $NaBH_4$ (0.4 mmol) in 40 mL of absolute ethanol. The solution turned dark red immediately upon addition of the reducing agent. The mixture was allowed to react over a period of 24 h until the completion of the reaction. The solution was then filtered. To the filtrate was added a solution of 0.1 mmol of $NaSbF_6$ in 10 mL of ethanol. The reaction mixture was allowed to stir for a few more minutes and was then refiltered. The dark brown-red product was recrystallized from ethanol/hexanes (ratio of ethanol/hexanes is approximately 5:1) by evaporation under nitrogen at room temperature (yield 27%). FTIR (Digilab FTS40) indicated the absence of SbF_6^-.

B. Collection and Reduction of X-ray Data. A dark-red prismatic crystal of dimensions 0.1 mm × 0.1 mm × 0.05 mm was selected and mounted in a glass capillary. Single-crystal X-ray diffraction data were collected on a Enraf-Nonius CAD4 diffractometer with use of graphite-monochromatized Mo Kα radiation (λ = 0.7107 Å). Details of the crystal parameters and data collection are summarized in Table I. The diffraction pattern was relatively weak and did not extend beyond $2\theta > 46°$. A complete set of data was collected from three crystals over a period of 1 month. For the four octants with $2° \le 2\theta \le 46°$, 64687 reflections were measured, after merging from three parts of collected data (part I, 2–20°, crystal 1; part II, 2–20°, crystal 2; part III, 20–23°, crystal 3). It yielded 14349 independent reflections with $I > 1\sigma(I)$ after equivalent reflections were averaged by using the program PAINT of the SDP package. A decay correction (using program CHORT) was made on each part of the collected data. The observed intensities were corrected for Lorentz and polarization effects but not for absorption since the ψ scan data were collected after the crystals had deteriorated. No extinction correction was made. The centrosymmetric space group $P\bar{1}$ (No. 2) was confirmed by successful solution and refinement of the structure. Since the center of the cluster (0.486, 0.179, 0.306) is in a general position (viz., $x, y, z; -x, -y, -z$), the analysis required the location of 18 Au, 20 Ag, 14 Cl, and 12 $(Tol)_3P$ groups in an asymmetric unit, or equivalently, two clusters (Z = 2) per unit cell.

C. Solution and Refinement of the Structure. 1. Direct Method and Fourier Syntheses. The positions of the metal atoms were obtained from direct methods, and the Cl and P atoms were located via Fourier syntheses. The majority of the tolyl carbon atoms were located from subsequent difference Fourier syntheses. The missing tolyl carbon atoms were then inferred from the known geometry and the resulting tolyl groups refined as rigid bodies (see the next section). Least-squares refinements of the metal core (the tolyl carbon atoms were included in the calculations but not refined) gave discrepancy factors of $R_1 = [\sum||F_o| - |F_c||/\sum|F_o|] \times 100\% = 15.2\%$, $R_2 = [\sum w_i||F_o| - |F_c||^2/\sum w_i|F_o|^2]^{1/2} \times 100\% = 18.8\%$ where $w_i = 1/\sigma_i^2(F_o)$.

2. Rigid-Body Refinement of Tolyl Groups. Rigid-body constraints were applied to all 12 tolyl groups with ring C–C distances of 1.39 Å, C–CH_3 distance of 1.47 Å, and a uniform isotropic temperature factor. Tolyl groups were numbered as TY*i*A, TY*i*B, and TY*i*C for tolyl groups A, B, and C, respectively, of the *i*th phosphine ligand, P*i* (i = 1–12).

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Table II. Selected Interatomic Distances (Å) and Their Estimated Standard Deviations for Cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$[a]

atom 1	atom 2	distance	atom 1	atom 2	distance	atom 1	atom 2	distance	atom 1	atom 2	distance
Au1	Au2	3.08 (1)	Au9	Au15	2.685 (9)	Au16	Ag6	2.88 (1)	Ag8	Cl8	3.13 (4)
Au1	Au7	2.96 (1)	Au9	Ag3	2.89 (1)	Au16	Ag7	2.89 (1)	Ag9	Ag10	2.90 (2)
Au1	Au8	2.92 (1)	Au9	Ag5	3.03 (1)	Au16	Ag8	2.95 (1)	Ag9	Ag11	3.10 (1)
Au1	Au13	2.78 (1)	Au9	Ag15	2.85 (1)	Au16	Ag15	3.09 (1)	Ag9	Ag17	2.83 (2)
Au1	Ag11	2.95 (1)	Au9	P9	2.30 (4)	Au16	Ag16	2.83 (1)	Ag9	Cl9	2.45 (4)
Au1	Ag12	2.95 (1)	Au10	Au15	2.685 (8)	Au16	Ag17	2.82 (1)	Ag9	Cl11	3.03 (4)
Au1	P1	2.41 (6)	Au10	Ag4	3.04 (1)	Au16	Ag18	3.01 (2)	Ag10	Ag12	3.09 (1)
Au2	Au7	2.878 (9)	Au10	Ag6	2.89 (1)	Au17	Au18	2.843 (8)	Ag10	Ag18	2.95 (2)
Au2	Au8	2.934 (9)	Au10	Ag16	2.86 (2)	Au17	Ag7	2.78 (1)	Ag10	Cl10	2.44 (4)
Au2	Au13	2.744 (7)	Au10	P10	2.29 (4)	Au17	Ag8	2.79 (1)	Ag11	Ag12	2.89 (2)
Au2	Ag1	2.98 (1)	Au11	Au17	2.719 (8)	Au17	Ag9	2.75 (1)	Ag11	Ag13	2.91 (2)
Au2	Ag2	2.95 (1)	Au11	Ag7	2.90 (1)	Au17	Ag10	2.80 (1)	Ag11	Cl9	2.47 (4)
Au2	P2	2.38 (4)	Au11	Ag9	3.02 (1)	Au17	Ag17	2.82 (1)	Ag12	Ag14	2.83 (2)
Au3	Au4	3.059 (9)	Au11	Ag17	2.89 (1)	Au17	Ag18	2.80 (1)	Ag12	Cl10	2.44 (4)
Au3	Au9	2.94 (1)	Au11	P11	2.34 (4)	Au18	Ag9	2.89 (1)	Ag12	Cl12	3.14 (3)
Au3	Au10	2.87 (1)	Au12	Au17	2.698 (8)	Au18	Ag10	2.87 (2)	Ag13	Ag15	3.24 (2)
Au3	Au15	2.76 (1)	Au12	Ag8	3.04 (2)	Au18	Ag11	2.88 (1)	Ag13	Ag17	3.22 (1)
Au3	Ag3	2.96 (1)	Au12	Ag10	2.91 (1)	Au18	Ag12	2.91 (2)	Ag13	Cl3	2.73 (4)
Au3	Ag4	2.98 (2)	Au12	Ag18	2.89 (1)	Au18	Ag13	2.86 (1)	Ag13	Cl11	2.55 (4)
Au3	P3	2.47 (4)	Au12	P12	2.31 (4)	Au18	Ag14	3.08 (1)	Ag14	Ag16	3.11 (2)
Au4	Au9	2.880 (9)	Au13	Au14	2.87 (1)	Au18	Ag17	3.08 (1)	Ag14	Ag18	3.19 (1)
Au4	Au10	2.95 (1)	Au13	Au18	2.864 (8)	Au18	Ag18	2.82 (1)	Ag14	Cl4	2.56 (4)
Au4	Au15	2.77 (1)	Au13	Ag1	2.80 (1)	Ag1	Ag2	2.85 (2)	Ag14	Cl12	2.73 (4)
Au4	Ag5	3.00 (2)	Au13	Ag2	2.77 (1)	Ag1	Ag3	3.18 (2)	Ag15	Ag17	3.09 (2)
Au4	Ag6	2.97 (2)	Au13	Ag11	2.79 (1)	Ag1	Ag13	2.86 (1)	Ag15	Cl3	2.63 (3)
Au4	P4	2.36 (4)	Au13	Ag12	2.74 (1)	Ag1	Cl1	2.35 (5)	Ag15	Cl7	2.71 (4)
Au5	Au6	3.10 (1)	Au13	Ag13	2.82 (1)	Ag1	Cl3	3.18 (4)	Ag16	Ag18	3.19 (2)
Au5	Au11	2.934 (9)	Au13	Ag14	2.82 (1)	Ag2	Ag4	3.11 (2)	Ag16	Cl4	2.71 (3)
Au5	Au12	2.90 (1)	Au14	Au15	2.86 (1)	Ag2	Ag14	2.93 (1)	Ag16	Cl8	2.60 (4)
Au5	Au17	2.739 (7)	Au14	Au16	2.86 (1)	Ag2	Cl2	2.42 (4)	Ag17	Cl7	2.56 (5)
Au5	Ag7	2.94 (1)	Au14	Au18	2.83 (1)	Ag3	Ag4	2.87 (2)	Ag17	Cl11	2.70 (3)
Au5	Ag8	2.95 (1)	Au14	Ag1	2.96 (1)	Ag3	Ag15	2.92 (2)	Ag18	Cl8	2.69 (4)
Au5	P5	2.35 (3)	Au14	Ag2	2.89 (1)	Ag3	Cl1	2.50 (4)	Ag18	Cl12	2.51 (4)
Au6	Au11	2.93 (1)	Au14	Ag3	2.88 (2)	Ag4	Ag16	2.86 (1)	Ag19	Cl3	2.53 (4)
Au6	Au12	2.95 (1)	Au14	Ag4	2.90 (2)	Ag4	Cl2	2.51 (3)	Ag19	Cl7	2.59 (4)
Au6	Au17	2.76 (1)	Au14	Ag13	3.07 (1)	Ag4	Cl4	3.18 (4)	Ag19	Cl11	2.66 (5)
Au6	Ag9	2.96 (1)	Au14	Ag14	2.85 (2)	Ag5	Ag6	2.89 (2)	Ag19	Cl13	2.38 (5)
Au6	Ag10	2.93 (1)	Au14	Ag15	2.86 (1)	Ag5	Ag7	3.11 (2)	Ag20	Cl4	2.67 (3)
Au6	P6	2.43 (5)	Au14	Ag16	3.07 (1)	Ag5	Ag15	2.83 (1)	Ag20	Cl8	2.53 (4)
Au7	Au13	2.691 (8)	Au15	Au16	2.86 (1)	Ag5	Cl5	2.53 (3)	Ag20	Cl12	2.65 (4)
Au7	Ag1	3.04 (1)	Au15	Ag3	2.80 (1)	Ag5	Cl7	3.21 (4)	Ag20	Cl14	2.37 (5)
Au7	Ag11	2.88 (1)	Au15	Ag4	2.79 (1)	Ag6	Ag8	3.20 (2)	Ag19	Ag13	3.76 (2)
Au7	Ag13	2.85 (1)	Au15	Ag5	2.76 (1)	Ag6	Ag16	2.92 (1)	Ag19	Ag15	3.70 (2)
Au7	P7	2.31 (4)	Au15	Ag6	2.79 (1)	Ag6	Cl6	2.47 (3)	Ag19	Ag17	3.69 (2)
Au8	Au13	2.706 (8)	Au15	Ag15	2.81 (1)	Ag7	Ag8	2.87 (2)	Ag20	Ag14	3.80 (2)
Au8	Ag2	2.91 (2)	Au15	Ag16	2.82 (1)	Ag7	Ag17	2.89 (1)	Ag20	Ag16	3.69 (2)
Au8	Ag12	3.01 (1)	Au16	Au17	2.86 (1)	Ag7	Cl5	2.44 (5)	Ag20	Ag18	3.76 (2)
Au8	Ag14	2.88 (1)	Au16	Au18	2.82 (1)	Ag8	Ag18	2.86 (1)			
Au8	P8	2.32 (4)	Au16	Ag5	2.91 (2)	Ag8	Cl6	2.39 (4)			

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

Individual carbons are numbered as C*imj* (where $i = 1$–12, m = A–C, and $j = 1$–7) for the C*j* carbon of the *m*th tolyl group bonded to the *i*th phosphine ligand. The position and orientation of the tolyl groups were refined with the group positional parameters x, y, z (in fractional coordinates) and orientation parameterss ϕ, θ, ρ (in degrees), respectively. The discrepancy factors at this point were $R_1 = 13.8\%$, $R_2 = 15.2\%$.

3. Disordered Solvent Atoms. All solvent molecules, as revealed by difference Fourier syntheses, are highly disordered. The following strategy of least-squares refinements was adopted. First, the occupancy factors of the solvent atoms were refined by using an isotropic thermal parameter of $B = 8$ Å^2 (roughly the average of the tolyl groups). The refined occupancy factors of these atoms were then fixed while their thermal parameters (B's) were being refined along with all heavy atoms (refining positional and thermal parameters) and all tolyl groups (included in the calculations but not refined).

4. Final Cycles of Refinement. In the final cycles of the refinement, anisotropic thermal parameters were used for heavy atoms (Au, Ag, Cl, and P) while the highly disordered solvent atoms were refined isotropically. Tolyl atoms, already refined as rigid-body groups as described in II.C.2, were not refined but included in the calculations. Final $R_1 = [\sum||F_o| - |F_c||/\sum|F_o|] \times 100\%$ and $R_2 = [\sum w_i||F_o| - |F_c||^2/\sum w_i|F_o|^2]^{1/2} \times 100\%$ values were 10.1% and 11.8%, respectively, for 8150 unique reflections with $I > 3\sigma(I)$ and 581 variables. After a final full-matrix refinement, a difference map showed no peaks >1.0 electron Å^3 (except near heavy atoms). Final atomic coordinates and thermal parameters with the estimated standard deviations of cluster **1** (heavy atoms only) are presented in Table A and Table B (supplementary material), respectively. The final positional and thermal parameters from the output of the last cycle of constrained least-squares refinement of cluster **1** for each group ($x, y, z, \phi, \theta, \rho$, and B) and for individual tolyl ring-carbon atoms (x, y, z, and B) are listed in Table C and Table D (supplementary material), respectively. Also given in Table C are the internal coordinates of the tolyl groups. The results of the positional and thermal parameters with the refined occupancy factors of solvent atoms are summarized in Table E (supplementary material). Selected interatomic distances and bond angles, together with the estimated standard deviations, are given in Tables II and III, respectively. Least-squares calculations of "best" molecular planes formed by certain groups of atoms and the perpendicular distance of these and other atoms from those planes are summarized in Table F (supplementary material). Selected intra- and intermolecular van der Waals contacts are listed in Table G (supplementary material). Observed and calculated structure factors are listed in Table H (supplementary material).

(III) Results and Discussion

A. Cluster Architecture. The $[Au_{18}Ag_{20}]$ and $[P_{12}Au_{18}Ag_{20}Cl_{14}]$ frameworks of cluster **1**, which conform to idealized D_{3h} symmetry, are portrayed in Figure 1, parts a and b, respectively. The most obvious description of the structure is as three 13-atom (Au_7Ag_6) Au-centered icosahedra sharing three Au vertices in a cyclic

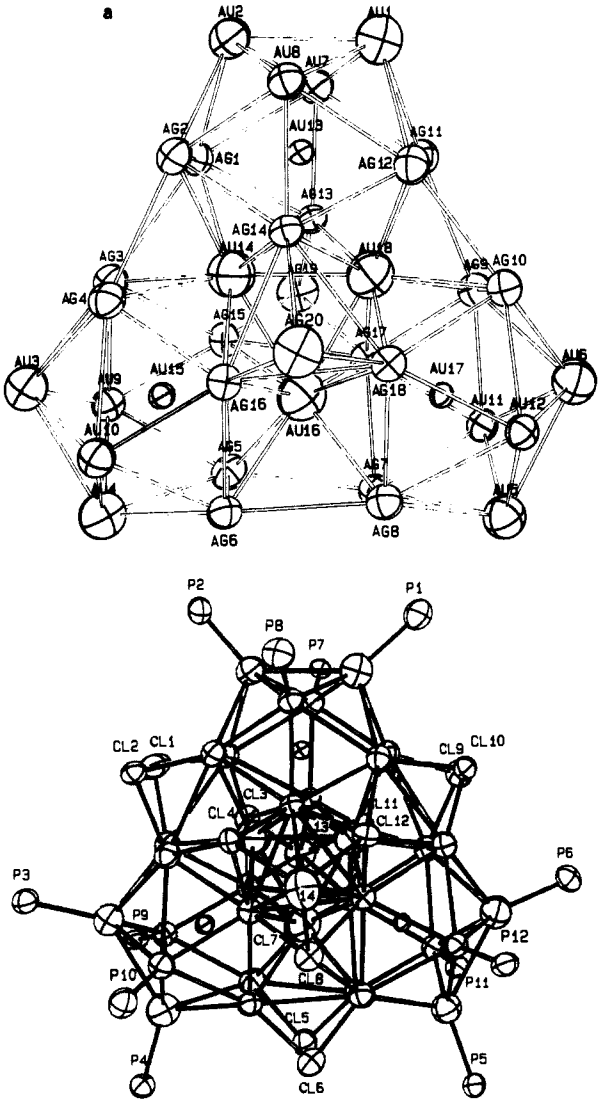

Figure 1. (a) $[Au_{18}Ag_{20}]$ framework of cluster **1** depicting three 13-atom (Au_7Ag_6) Au-centered icosahedra sharing three Au vertices in a cyclic manner plus two capping Ag atoms (Ag19 and Ag20) located on the idealized 3-fold axis. (b) $[P_{12}Au_{18}Ag_{20}Cl_{14}]$ framework of cluster **1**. All bonds radiating from the centers of the icosahedra (Au13, Au15, and Au17) are omitted for clarity. In (b), Cl13 and Cl14 are designated 13 and 14, respectively, for clarity.

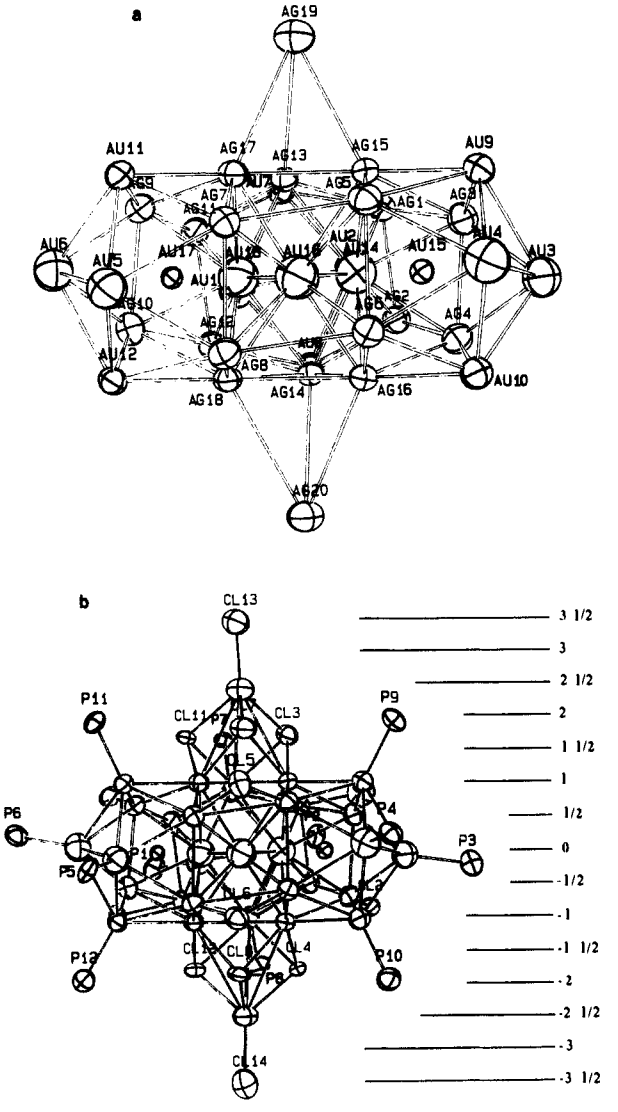

Figure 2. Side views of (a) the metal framework $[Au_{18}Ag_{20}]$ and (b) the $[P_{12}Au_{18}Ag_{20}Cl_{14}]$ framework of cluster **1**. Also shown in (b) is a labeling system for the approximate layers.

manner plus two capping Ag atoms located on the idealized 3-fold axis. As such, the 18 Au atoms can be divided into two categories: 12 on the surface (Au1–Au12) and 6 in the interior. The six interior gold atoms include the icosahedral centers Au13, Au15, and Au17 and the shared vertices Au14, Au16, and Au18. The 20 Ag atoms can be classified into three types (with decreasing distance from the idealized 3-fold symmetry axis of the cluster): 12 on the peripherals (type A Ag1–Ag12), 6 in the center (type B Ag13–Ag18), and 2 on the idealized 3-fold axis (type C Ag19 and Ag20).

A second description of the metal framework is based on close packing of metal atoms (cf. Figure 2 of ref 3b). In this description, imagine a two-dimensional arrangement of 12 Au atoms, forming a ν_2 triangle and three ν_1 triangles sharing corners. Above and below the three small triangles are six Au atoms conceptually changing the smaller triangles into trigonal bipyramids. Above and below the central (large) triangle are eight Ag atoms arranged in two tetrahedral arrays, which are connected by an elongated and distorted trigonal prism. Further addition of three distorted squares of Ag atoms (total of 12) to the three square faces of the distorted trigonal prism completes the arrangement of the 20 Ag atoms in the cluster.

Yet a third description of the structure is that it can be considered as three interpenetrating 25-atom clusters. Thus, if one views along the pseudo-5-fold axes marked by an arrow in Figure 2 of ref 3b, the same 1:5:1:5:1:5:1:5:1 structural arrangement of metal atoms can be seen. (Note, however, that the four pentagons are arranged in a *s–e–s* configuration in the 25-atom cluster, where *s* and *e* denote staggered and eclipsed, respectively.) The structure is completed by two "apical" Ag atoms located on the idealized 3-fold axis.

The side views of the $[Au_{18}Ag_{20}]$ and the $[P_{12}Au_{18}Ag_{20}Cl_{14}]$ frameworks of cluster **1** are portrayed in Figure 2, parts a and b, respectively. A labeling system for the approximate layer arrangement of the heavy atoms is also indicated in Figure 2b.

B. Cluster Parameters. Considering the *metal framework* of cluster **1**, the 18 Au atoms fall into two distinct classes exhibiting different coordination patterns: the central ν_2 triangle Au atoms (Au13–Au18), which are perpendicular to the 3-fold axis, are twelve-coordinate, the peripheral Au atoms, which form a highly distorted twinned cuboctahedron, are six-coordinate. The 20 Ag atoms can also be categorized into three groups in terms of coordination patterns: type A, B, and C Ag atoms are seven-, eight-, and zero-coordinate, respectively (see next paragraph). Here we consider only metal–metal contacts.

The metal–metal distances follow the approximate trend Au–Au (2.69–3.09 Å) ~ Au–Ag (2.75–3.09) < Ag–Ag (2.84–3.24 Å), all of which can be considered as more or less bonding. There are four groups of Ag–Ag distances: 2.83–2.95 Å for unbridged, 3.09–3.20 Å for doubly bridged and 3.09–3.24 Å for triply bridged Ag–Ag bonds. The Ag···Ag contacts of 3.69–3.80 Å involving

Table III. Selected Bond Angles (deg) and Their Estimated Standard Deviations for Cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$[a]

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
Au2	Au1	Au7	56.8 (3)	Ag5	Au4	Ag6	57.8 (4)	Ag2	Au8	Ag12	105.4 (4)	Au17	Au12	Ag10	59.7 (3)
Au2	Au1	Au8	58.4 (3)	Ag5	Au4	P4	114 (1)	Ag2	Au8	Ag14	60.6 (3)	Au17	Au12	Ag18	60.2 (3)
Au2	Au1	Au13	55.5 (2)	Ag6	Au4	P4	114 (1)	Ag2	Au8	P8	120 (1)	Au17	Au12	P12	179.3 (9)
Au2	Au1	Ag11	104.6 (4)	Au6	Au5	Au11	58.1 (2)	Ag12	Au8	Ag14	57.4 (3)	Ag8	Au12	Ag10	107.1 (4)
Au2	Au1	Ag12	106.1 (4)	Au6	Au5	Au12	58.9 (2)	Ag12	Au8	P8	125 (1)	Ag8	Au12	Ag18	57.7 (3)
Au2	Au1	P1	138 (1)	Au6	Au5	Au17	56.0 (2)	Ag14	Au8	P8	120 (1)	Ag8	Au12	P12	123 (1)
Au7	Au1	Au8	103.7 (4)	Au6	Au5	Ag7	105.7 (4)	Au3	Au9	Au4	63.3 (2)	Ag10	Au12	Ag18	61.1 (4)
Au7	Au1	Au13	55.8 (3)	Au6	Au5	Ag8	108.0 (3)	Au3	Au9	Au15	58.5 (2)	Ag10	Au12	P12	120 (1)
Au7	Au1	Ag11	58.5 (3)	Au6	Au5	P5	133 (1)	Au3	Au9	Ag3	61.0 (4)	Ag18	Au12	P12	119 (1)
Au7	Au1	Ag12	104.0 (4)	Au11	Au5	Au12	105.8 (2)	Au3	Au9	Ag5	109.3 (3)	Au1	Au13	Au2	67.8 (3)
Au7	Au1	P1	127 (1)	Au11	Au5	Au17	57.2 (2)	Au3	Au9	Ag15	110.4 (4)	Au1	Au13	Au7	65.5 (3)
Au8	Au1	Au13	56.6 (3)	Au11	Au5	Ag7	59.2 (3)	Au3	Au9	P9	123 (1)	Au1	Au13	Au8	64.4 (3)
Au8	Au1	Ag11	107.6 (4)	Au11	Au5	Ag8	106.0 (3)	Au4	Au9	Au15	59.5 (3)	Au1	Au13	Au14	173.3 (3)
Au8	Au1	Ag12	61.7 (3)	Au11	Au5	P5	127 (1)	Au4	Au9	Ag3	112.3 (4)	Au1	Au13	Au18	115.7 (3)
Au8	Au1	P1	127 (1)	Au12	Au5	Au17	57.1 (2)	Au4	Au9	Ag5	60.8 (3)	Au1	Au13	Ag1	123.7 (3)
Au13	Au1	Ag11	58.3 (3)	Au12	Au5	Ag7	107.9 (3)	Au4	Au9	Ag15	109.7 (3)	Au1	Au13	Ag2	120.5 (3)
Au13	Au1	Ag12	57.1 (4)	Au12	Au5	Ag8	62.7 (3)	Au4	Au9	P9	122 (1)	Au1	Au13	Ag11	63.8 (3)
Au13	Au1	P1	166.1 (9)	Au12	Au5	P5	123 (1)	Au15	Au9	Ag3	60.0 (3)	Au1	Au13	Ag12	64.5 (3)
Ag11	Au1	Ag12	58.7 (3)	Au17	Au5	Ag7	58.6 (3)	Au15	Au9	Ag5	57.5 (3)	Au1	Au13	Ag13	116.8 (4)
Ag11	Au1	P1	110 (1)	Au17	Au5	Ag8	58.7 (3)	Au15	Au9	Ag15	61.0 (3)	Au1	Au13	Ag14	114.5 (4)
Ag12	Au1	P1	111 (1)	Au17	Au5	P5	171 (1)	Au15	Au9	P9	178 (1)	Au2	Au13	Au7	63.9 (2)
Au1	Au2	Au7	59.4 (3)	Ag7	Au5	Ag8	58.4 (3)	Ag3	Au9	Ag5	106.5 (4)	Au2	Au13	Au8	65.1 (2)
Au1	Au2	Au8	58.1 (2)	Ag7	Au5	P5	115 (1)	Ag3	Au9	Ag15	61.2 (4)	Au2	Au13	Au14	117.7 (3)
Au1	Au2	Au13	56.7 (2)	Ag8	Au5	P5	112 (1)	Ag3	Au9	P9	118.8 (8)	Au2	Au13	Au18	174.4 (3)
Au1	Au2	Ag1	108.5 (3)	Au5	Au6	Au11	58.1 (2)	Ag5	Au9	Ag15	57.3 (3)	Au2	Au13	Ag1	65.1 (3)
Au1	Au2	Ag2	105.9 (3)	Au5	Au6	Au12	57.1 (2)	Ag5	Au9	P9	122.1 (9)	Au2	Au13	Ag2	64.7 (3)
Au1	Au2	P2	133 (1)	Au5	Au6	Au17	55.3 (3)	Ag15	Au9	P9	117 (1)	Au2	Au13	Ag11	118.9 (3)
Au7	Au2	Au8	105.5 (3)	Au5	Au6	Ag9	105.7 (4)	Au3	Au10	Au4	63.3 (2)	Au2	Au13	Ag12	122.9 (3)
Au7	Au2	Au13	57.1 (2)	Au5	Au6	Ag10	105.3 (4)	Au3	Au10	Au15	59.4 (2)	Au2	Au13	Ag13	114.4 (3)
Au7	Au2	Ag1	62.5 (3)	Au5	Au6	P6	142.7 (8)	Au3	Au10	Ag4	60.4 (3)	Au2	Au13	Ag14	117.5 (3)
Au7	Au2	Ag2	107.0 (3)	Au11	Au6	Au12	104.3 (3)	Au3	Au10	Ag6	112.2 (4)	Au7	Au13	Au8	118.1 (2)
Au7	Au2	P2	121 (1)	Au11	Au6	Au17	57.0 (2)	Au3	Au10	Ag16	109.5 (3)	Au7	Au13	Au14	119.9 (3)
Au8	Au2	Au13	56.8 (2)	Au11	Au6	Ag9	61.6 (3)	Au3	Au10	P10	123 (1)	Au7	Au13	Au18	112.9 (2)
Au8	Au2	Ag1	105.4 (3)	Au11	Au6	Ag10	108.3 (4)	Au4	Au10	Au15	58.5 (2)	Au7	Au13	Ag1	67.3 (4)
Au8	Au2	Ag2	59.4 (3)	Au11	Au6	P6	124 (1)	Au4	Au10	Ag4	109.5 (3)	Au7	Au13	Ag2	118.3 (3)
Au8	Au2	P2	130 (1)	Au12	Au6	Au17	56.2 (2)	Au4	Au10	Ag6	61.1 (3)	Au7	Au13	Ag11	63.4 (3)
Au13	Au2	Ag1	58.4 (3)	Au12	Au6	Ag9	104.8 (3)	Au4	Au10	Ag16	110.4 (4)	Au7	Au13	Ag12	117.9 (4)
Au13	Au2	Ag2	58.0 (3)	Au12	Au6	Ag10	59.3 (3)	Au4	Au10	P10	122 (1)	Au7	Au13	Ag13	62.4 (3)
Au13	Au2	P2	169 (1)	Au12	Au6	P6	131 (1)	Au15	Au10	Ag4	57.9 (3)	Au7	Au13	Ag14	178.5 (3)
Ag1	Au2	Ag2	57.4 (4)	Au17	Au6	Ag9	57.2 (3)	Au15	Au10	Ag6	59.9 (3)	Au8	Au13	Au14	113.6 (3)
Ag1	Au2	P2	111 (1)	Au17	Au6	Ag10	58.9 (4)	Au15	Au10	Ag16	60.9 (3)	Au8	Au13	Au18	120.1 (3)
Ag2	Au2	P2	117 (1)	Au17	Au6	P6	161.7 (9)	Au15	Au10	P10	178 (1)	Au8	Au13	Ag1	117.4 (3)
Au4	Au3	Au9	57.3 (2)	Ag9	Au6	Ag10	59.0 (3)	Ag4	Au10	Ag6	107.0 (4)	Au8	Au13	Ag2	64.4 (3)
Au4	Au3	Au10	59.7 (2)	Ag9	Au6	P6	105.8 (9)	Ag4	Au10	Ag16	57.9 (3)	Au8	Au13	Ag11	118.9 (4)
Au4	Au3	Au15	56.5 (2)	Ag10	Au6	P6	108 (1)	Ag4	Au10	P10	122.3 (9)	Au8	Au13	Ag12	67.1 (3)
Au4	Au3	Ag3	105.5 (4)	Au1	Au7	Au2	63.7 (3)	Ag6	Au10	Ag16	60.9 (3)	Au8	Au13	Ag13	178.6 (4)
Au4	Au3	Ag4	108.4 (4)	Au1	Au7	Au13	58.7 (2)	Ag6	Au10	P10	118.5 (9)	Au8	Au13	Ag14	62.9 (3)
Au4	Au3	P3	133 (1)	Au1	Au7	Ag1	110.2 (4)	Ag16	Au10	P10	117 (1)	Au14	Au13	Au18	59.2 (3)
Au9	Au3	Au10	104.7 (3)	Au1	Au7	Ag11	60.5 (3)	Au5	Au11	Au6	63.8 (3)	Au14	Au13	Ag1	63.0 (3)
Au9	Au3	Au15	56.1 (2)	Au1	Au7	Ag13	110.2 (3)	Au5	Au11	Au17	57.8 (2)	Au14	Au13	Ag2	61.6 (3)
Au9	Au3	Ag3	58.7 (3)	Au1	Au7	P7	124 (1)	Au5	Au11	Ag7	60.4 (3)	Au14	Au13	Ag11	114.0 (3)
Au9	Au3	Ag4	104.3 (4)	Au2	Au7	Au13	58.9 (2)	Au5	Au11	Ag9	108.5 (3)	Au14	Au13	Ag12	108.8 (3)
Au9	Au3	P3	129 (1)	Au2	Au7	Ag1	60.5 (3)	Au5	Au11	Ag17	108.8 (3)	Au14	Au13	Ag13	65.3 (3)
Au10	Au3	Au15	56.9 (2)	Au2	Au7	Ag11	111.7 (3)	Au5	Au11	P11	121.0 (8)	Au14	Au13	Ag14	60.0 (3)
Au10	Au3	Ag3	107.6 (4)	Au2	Au7	Ag13	109.2 (3)	Au6	Au11	Au17	58.3 (2)	Au18	Au13	Ag1	109.6 (3)
Au10	Au3	Ag4	62.7 (3)	Au2	Au7	P7	122.4 (9)	Au6	Au11	Ag7	111.2 (4)	Au18	Au13	Ag2	114.9 (3)
Au10	Au3	P3	123.4 (9)	Au13	Au7	Ag1	58.1 (3)	Au6	Au11	Ag9	59.6 (3)	Au18	Au13	Ag11	61.2 (3)
Au15	Au3	Ag3	58.4 (3)	Au13	Au7	Ag11	60.0 (3)	Au6	Au11	Ag17	107.9 (3)	Au18	Au13	Ag12	62.5 (3)
Au15	Au3	Ag4	58.1 (3)	Au13	Au7	Ag13	61.0 (3)	Au6	Au11	P11	122 (1)	Au18	Au13	Ag13	60.4 (3)
Au15	Au3	P3	170 (1)	Au13	Au7	P7	177 (1)	Au17	Au11	Ag7	59.3 (3)	Au18	Au13	Ag14	65.6 (3)
Ag3	Au3	Ag4	57.8 (4)	Ag1	Au7	Ag11	107.3 (3)	Au17	Au11	Ag9	56.9 (3)	Ag1	Au13	Ag2	61.5 (4)
Ag3	Au3	P3	114.8 (9)	Ag1	Au7	Ag13	58.0 (3)	Au17	Au11	Ag17	60.3 (3)	Ag1	Au13	Ag11	117.2 (4)
Ag4	Au3	P3	112 (1)	Ag1	Au7	P7	120 (1)	Au17	Au11	P11	178 (1)	Ag1	Au13	Ag12	171.5 (4)
Au3	Au4	Au9	59.4 (2)	Ag11	Au7	Ag13	61.0 (3)	Ag7	Au11	Ag9	105.1 (3)	Ag1	Au13	Ag13	61.3 (3)
Au3	Au4	Au10	57.0 (2)	Ag11	Au7	P7	120 (1)	Ag7	Au11	Ag17	59.9 (3)	Ag1	Au13	Ag14	113.5 (4)
Au3	Au4	Au15	56.3 (3)	Ag13	Au7	P7	116 (1)	Ag7	Au11	P11	119 (1)	Ag2	Au13	Ag11	175.7 (4)
Au3	Au4	Ag5	107.2 (3)	Au1	Au8	Au2	63.5 (3)	Ag9	Au11	Ag17	57.0 (3)	Ag2	Au13	Ag12	117.7 (4)
Au3	Au4	Ag6	104.9 (4)	Au1	Au8	Au13	59.1 (3)	Ag9	Au11	P11	124.7 (9)	Ag2	Au13	Ag13	114.2 (4)
Au3	Au4	P4	134 (1)	Au1	Au8	Ag2	111.2 (4)	Ag17	Au11	P11	120 (1)	Ag2	Au13	Ag14	63.1 (3)
Au9	Au4	Au10	104.2 (3)	Au1	Au8	Ag12	59.5 (3)	Au5	Au12	Au6	64.1 (3)	Ag11	Au13	Ag12	62.8 (4)
Au9	Au4	Au15	56.7 (3)	Au1	Au8	Ag14	108.5 (3)	Au5	Au12	Au17	58.5 (2)	Ag11	Au13	Ag13	62.6 (4)
Au9	Au4	Ag5	62.1 (3)	Au1	Au8	P8	121 (1)	Au5	Au12	Ag8	59.5 (3)	Ag11	Au13	Ag14	115.1 (3)
Au9	Au4	Ag6	107.2 (4)	Au2	Au8	Au13	58.1 (2)	Au5	Au12	Ag10	111.3 (4)	Ag12	Au13	Ag13	114.0 (4)
Au9	Au4	P4	125 (1)	Au2	Au8	Ag2	60.6 (3)	Au5	Au12	Ag18	107.8 (4)	Ag12	Au13	Ag14	61.2 (4)
Au10	Au4	Au15	55.9 (3)	Au2	Au8	Ag12	108.3 (3)	Au5	Au12	P12	122.2 (9)	Ag13	Au13	Ag14	116.7 (3)
Au10	Au4	Ag5	103.7 (4)	Au2	Au8	Ag14	109.8 (3)	Au6	Au12	Au17	58.3 (2)	Au13	Au14	Au15	178.6 (4)
Au10	Au4	Ag6	58.4 (3)	Au2	Au8	P8	120.1 (9)	Au6	Au12	Ag8	109.5 (3)	Au13	Au14	Au16	119.8 (4)
Au10	Au4	P4	127 (1)	Au13	Au8	Ag2	58.8 (3)	Au6	Au12	Ag10	59.9 (3)	Au13	Au14	Au18	60.4 (3)
Au15	Au4	Ag5	57.2 (3)	Au13	Au8	Ag12	57.0 (3)	Au6	Au12	Ag18	109.2 (3)	Au13	Au14	Ag1	57.5 (3)
Au15	Au4	Ag6	58.0 (3)	Au13	Au8	Ag14	60.5 (3)	Au6	Au12	P12	122 (1)	Au13	Au14	Ag2	57.5 (3)
Au15	Au4	P4	170 (1)	Au13	Au8	P8	178 (1)	Au17	Au12	Ag8	57.9 (3)	Au13	Au14	Ag3	122.4 (3)

Table III (Continued)

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
Au13	Au14	Ag4	121.3 (4)	Au9	Au15	Au10	118.0 (3)	Au18	Au16	Ag17	66.1 (4)	Ag7	Au17	Ag8	61.9 (4)
Au13	Au14	Ag13	56.5 (3)	Au9	Au15	Au14	113.2 (3)	Au18	Au16	Ag18	57.6 (3)	Ag7	Au17	Ag9	116.4 (4)
Au13	Au14	Ag14	59.2 (3)	Au9	Au15	Au16	120.3 (3)	Ag5	Au16	Ag6	59.7 (4)	Ag7	Au17	Ag10	175.7 (4)
Au13	Au14	Ag15	122.4 (4)	Au9	Au15	Ag3	63.7 (3)	Ag5	Au16	Ag7	64.8 (4)	Ag7	Au17	Ag17	62.1 (3)
Au13	Au14	Ag16	122.1 (4)	Au9	Au15	Ag4	117.4 (3)	Ag5	Au16	Ag8	102.5 (4)	Ag7	Au17	Ag18	114.1 (4)
Au15	Au14	Au16	60.1 (3)	Au9	Au15	Ag5	67.6 (3)	Ag5	Au16	Ag15	56.1 (3)	Ag8	Au17	Ag9	171.0 (4)
Au15	Au14	Au18	119.5 (3)	Au9	Au15	Ag6	118.8 (3)	Ag5	Au16	Ag16	108.7 (5)	Ag8	Au17	Ag10	117.9 (4)
Au15	Au14	Ag1	123.5 (4)	Au9	Au15	Ag15	62.4 (3)	Ag5	Au16	Ag17	83.2 (4)	Ag8	Au17	Ag17	112.8 (4)
Au15	Au14	Ag2	122.0 (4)	Au9	Au15	Ag16	178.4 (3)	Ag5	Au16	Ag18	158.4 (4)	Ag8	Au17	Ag18	61.5 (3)
Au15	Au14	Ag3	58.4 (3)	Au10	Au15	Au14	119.6 (3)	Ag6	Au16	Ag7	85.0 (4)	Ag9	Au17	Ag10	63.1 (4)
Au15	Au14	Ag4	57.9 (3)	Au10	Au15	Au16	113.0 (3)	Ag6	Au16	Ag8	66.5 (4)	Ag9	Au17	Ag17	61.0 (4)
Au15	Au14	Ag13	124.7 (4)	Au10	Au15	Ag3	118.3 (3)	Ag6	Au16	Ag15	104.6 (5)	Ag9	Au17	Ag18	114.2 (3)
Au15	Au14	Ag14	119.5 (4)	Au10	Au15	Ag4	67.5 (3)	Ag6	Au16	Ag16	61.4 (4)	Ag10	Au17	Ag17	115.2 (3)
Au15	Au14	Ag15	58.9 (3)	Au10	Au15	Ag5	118.3 (3)	Ag6	Au16	Ag17	138.4 (5)	Ag10	Au17	Ag18	63.4 (4)
Au15	Au14	Ag16	56.6 (3)	Au10	Au15	Ag6	63.8 (3)	Ag6	Au16	Ag18	101.7 (4)	Ag17	Au17	Ag18	115.6 (3)
Au16	Au14	Au18	59.4 (3)	Au10	Au15	Ag15	178.9 (3)	Ag7	Au16	Ag8	58.9 (3)	Au13	Au18	Au14	60.4 (3)
Au16	Au14	Ag1	145.7 (4)	Au10	Au15	Ag16	62.7 (3)	Ag7	Au16	Ag15	99.5 (4)	Au13	Au18	Au16	121.2 (4)
Au16	Au14	Ag2	153.9 (4)	Au14	Au15	Au16	59.9 (3)	Ag7	Au16	Ag16	140.6 (4)	Au13	Au18	Au17	178.3 (4)
Au16	Au14	Ag3	112.5 (4)	Au14	Au15	Ag3	61.2 (3)	Ag7	Au16	Ag17	60.8 (3)	Au13	Au18	Ag9	121.6 (4)
Au16	Au14	Ag4	106.0 (4)	Au14	Au15	Ag4	61.8 (3)	Ag7	Au16	Ag18	105.1 (4)	Au13	Au18	Ag10	119.7 (4)
Au16	Au14	Ag13	92.1 (3)	Au14	Au15	Ag5	109.1 (4)	Ag8	Au16	Ag15	156.3 (4)	Au13	Au18	Ag11	58.2 (3)
Au16	Au14	Ag14	94.2 (4)	Au14	Au15	Ag6	115.0 (4)	Ag8	Au16	Ag16	87.5 (4)	Au13	Au18	Ag12	56.7 (3)
Au16	Au14	Ag15	65.5 (3)	Au14	Au15	Ag15	60.6 (3)	Ag8	Au16	Ag17	108.3 (4)	Au13	Au18	Ag13	59.0 (3)
Au16	Au14	Ag16	57.0 (3)	Au14	Au15	Ag16	65.4 (3)	Ag8	Au16	Ag18	57.4 (3)	Au13	Au18	Ag14	56.5 (2)
Au18	Au14	Ag1	106.1 (4)	Au16	Au15	Ag3	114.9 (4)	Ag15	Au16	Ag16	108.0 (4)	Au13	Au18	Ag17	123.9 (4)
Au18	Au14	Ag2	112.2 (5)	Au16	Au15	Ag4	109.0 (4)	Ag15	Au16	Ag17	62.8 (4)	Au13	Au18	Ag18	120.9 (4)
Au18	Au14	Ag3	154.7 (4)	Au16	Au15	Ag5	62.3 (3)	Ag15	Au16	Ag18	145.2 (4)	Au14	Au18	Au16	60.7 (3)
Au18	Au14	Ag4	144.0 (4)	Au16	Au15	Ag6	61.4 (3)	Ag16	Au16	Ag17	158.2 (4)	Au14	Au18	Au17	121.3 (4)
Au18	Au14	Ag13	57.8 (3)	Au16	Au15	Ag15	66.1 (3)	Ag16	Au16	Ag18	66.0 (4)	Au14	Au18	Ag9	141.7 (5)
Au18	Au14	Ag14	65.7 (4)	Au16	Au15	Ag16	59.8 (3)	Ag17	Au16	Ag18	109.3 (5)	Au14	Au18	Ag10	156.6 (4)
Au18	Au14	Ag15	95.2 (4)	Ag3	Au15	Ag4	61.8 (3)	Au5	Au17	Au6	68.7 (3)	Au14	Au18	Ag11	112.4 (4)
Au18	Au14	Ag16	90.2 (4)	Ag3	Au15	Ag5	117.3 (4)	Au5	Au17	Au11	65.0 (2)	Au14	Au18	Ag12	105.3 (4)
Ag1	Au14	Ag2	58.3 (3)	Ag3	Au15	Ag6	176.1 (5)	Au5	Au17	Au12	64.4 (2)	Au14	Au18	Ag13	65.2 (3)
Ag1	Au14	Ag3	66.0 (4)	Ag3	Au15	Ag15	62.8 (3)	Au5	Au17	Au16	116.8 (3)	Au14	Au18	Ag14	57.4 (3)
Ag1	Au14	Ag4	101.8 (4)	Ag3	Au15	Ag16	114.7 (4)	Au5	Au17	Au18	174.1 (3)	Au14	Au18	Ag17	89.6 (4)
Ag1	Au14	Ag13	56.7 (3)	Ag4	Au15	Ag5	170.6 (5)	Au5	Au17	Ag7	64.2 (3)	Au14	Au18	Ag18	96.6 (4)
Ag1	Au14	Ag14	108.2 (4)	Ag4	Au15	Ag6	117.6 (4)	Au5	Au17	Ag8	64.4 (3)	Au16	Au18	Au17	60.6 (3)
Ag1	Au14	Ag15	87.1 (4)	Ag4	Au15	Ag15	113.3 (3)	Au5	Au17	Ag9	123.6 (3)	Au16	Au18	Ag9	105.4 (4)
Ag1	Au14	Ag16	156.9 (4)	Ag4	Au15	Ag16	61.5 (3)	Au5	Au17	Ag10	119.9 (3)	Au16	Au18	Ag10	113.2 (4)
Ag2	Au14	Ag3	84.9 (4)	Ag5	Au15	Ag6	62.6 (3)	Au5	Au17	Ag17	116.8 (3)	Au16	Au18	Ag11	156.4 (5)
Ag2	Au14	Ag4	65.1 (4)	Ag5	Au15	Ag15	60.9 (3)	Au5	Au17	Ag18	114.9 (3)	Au16	Au18	Ag12	142.4 (4)
Ag2	Au14	Ag13	103.8 (4)	Ag5	Au15	Ag16	113.4 (4)	Au6	Au17	Au11	64.8 (3)	Au16	Au18	Ag13	97.5 (4)
Ag2	Au14	Ag14	61.4 (3)	Ag6	Au15	Ag15	115.2 (3)	Au6	Au17	Au12	65.5 (3)	Au16	Au18	Ag14	90.0 (4)
Ag2	Au14	Ag15	140.0 (4)	Ag6	Au15	Ag16	62.8 (3)	Au6	Au17	Au16	173.4 (3)	Au16	Au18	Ag17	57.0 (3)
Ag2	Au14	Ag16	100.8 (4)	Ag15	Au15	Ag16	116.9 (4)	Au6	Au17	Au18	115.5 (3)	Au16	Au18	Ag18	64.7 (4)
Ag3	Au14	Ag4	59.5 (4)	Au14	Au16	Au15	60.0 (3)	Au6	Au17	Ag7	120.5 (3)	Au17	Au18	Ag9	57.2 (3)
Ag3	Au14	Ag13	101.1 (4)	Au14	Au16	Au17	119.9 (4)	Au6	Au17	Ag8	123.7 (3)	Au17	Au18	Ag10	58.7 (3)
Ag3	Au14	Ag14	139.2 (4)	Au14	Au16	Au18	59.8 (3)	Au6	Au17	Ag9	65.1 (3)	Au17	Au18	Ag11	120.3 (4)
Ag3	Au14	Ag15	61.2 (4)	Au14	Au16	Ag5	105.2 (4)	Au6	Au17	Ag10	63.5 (3)	Au17	Au18	Ag12	122.0 (4)
Ag3	Au14	Ag16	105.3 (4)	Au14	Au16	Ag6	112.2 (4)	Au6	Au17	Ag17	115.1 (3)	Au17	Au18	Ag13	121.4 (4)
Ag4	Au14	Ag13	157.2 (4)	Au14	Au16	Ag7	153.3 (4)	Au6	Au17	Ag18	117.6 (4)	Au17	Au18	Ag14	124.1 (3)
Ag4	Au14	Ag14	84.3 (4)	Au14	Au16	Ag8	146.0 (4)	Au11	Au17	Au12	118.2 (2)	Au17	Au18	Ag17	56.8 (3)
Ag4	Au14	Ag15	108.6 (5)	Au14	Au16	Ag15	57.4 (3)	Au11	Au17	Au16	113.4 (3)	Au17	Au18	Ag18	59.4 (3)
Ag4	Au14	Ag16	57.3 (3)	Au14	Au16	Ag16	65.3 (3)	Au11	Au17	Au18	120.1 (3)	Ag9	Au18	Ag10	60.5 (4)
Ag13	Au14	Ag14	108.5 (5)	Au14	Au16	Ag17	94.3 (3)	Au11	Au17	Ag7	63.6 (3)	Ag9	Au18	Ag11	64.9 (3)
Ag13	Au14	Ag15	66.2 (4)	Au14	Au16	Ag18	91.7 (4)	Au11	Au17	Ag8	116.9 (3)	Ag9	Au18	Ag12	104.8 (5)
Ag13	Au14	Ag16	145.2 (4)	Au15	Au16	Au17	178.0 (4)	Au11	Au17	Ag9	67.1 (3)	Ag9	Au18	Ag13	83.3 (4)
Ag14	Au14	Ag15	158.0 (4)	Au15	Au16	Au18	119.8 (3)	Au11	Au17	Ag10	118.8 (4)	Ag9	Au18	Ag14	160.0 (5)
Ag14	Au14	Ag16	63.4 (4)	Au15	Au16	Ag5	57.2 (3)	Au11	Au17	Ag17	62.9 (3)	Ag9	Au18	Ag17	56.4 (4)
Ag15	Au14	Ag16	107.9 (4)	Au15	Au16	Ag6	58.1 (3)	Au11	Au17	Ag18	177.6 (4)	Ag9	Au18	Ag18	109.5 (4)
Au3	Au15	Au4	67.2 (3)	Au15	Au16	Ag7	121.1 (4)	Au12	Au17	Au16	119.7 (3)	Ag10	Au18	Ag11	81.7 (4)
Au3	Au15	Au9	65.5 (3)	Au15	Au16	Ag8	123.8 (4)	Au12	Au17	Au18	113.0 (3)	Ag10	Au18	Ag12	64.8 (4)
Au3	Au15	Au10	63.6 (2)	Au15	Au16	Ag15	56.2 (3)	Au12	Au17	Ag7	118.7 (3)	Ag10	Au18	Ag13	137.0 (5)
Au3	Au15	Au14	116.3 (3)	Au15	Au16	Ag16	59.3 (3)	Au12	Au17	Ag8	67.3 (3)	Ag10	Au18	Ag14	101.9 (4)
Au3	Au15	Au16	173.7 (3)	Au15	Au16	Ag17	118.5 (4)	Au12	Au17	Ag9	118.8 (4)	Ag10	Au18	Ag17	106.0 (4)
Au3	Au15	Ag3	64.5 (3)	Au15	Au16	Ag18	124.8 (4)	Au12	Au17	Ag10	63.9 (3)	Ag10	Au18	Ag18	62.4 (4)
Au3	Au15	Ag4	64.9 (3)	Au17	Au16	Au18	60.1 (3)	Au12	Au17	Ag17	178.8 (3)	Ag11	Au18	Ag12	59.8 (4)
Au3	Au15	Ag5	123.9 (4)	Au17	Au16	Ag5	121.4 (4)	Au12	Au17	Ag18	63.3 (3)	Ag11	Au18	Ag13	61.0 (4)
Au3	Au15	Ag6	119.1 (3)	Au17	Au16	Ag6	122.9 (3)	Au16	Au17	Au18	59.3 (3)	Ag11	Au18	Ag14	105.2 (4)
Au3	Au15	Ag15	117.3 (3)	Au17	Au16	Ag7	57.9 (3)	Au16	Au17	Ag7	61.7 (3)	Ag11	Au18	Ag17	102.2 (4)
Au3	Au15	Ag16	114.3 (3)	Au17	Au16	Ag8	57.5 (3)	Au16	Au17	Ag8	62.9 (3)	Ag11	Au18	Ag18	138.1 (5)
Au4	Au15	Au9	63.8 (3)	Au17	Au16	Ag15	121.9 (4)	Au16	Au17	Ag9	108.3 (3)	Ag12	Au18	Ag13	107.9 (4)
Au4	Au15	Au10	65.6 (3)	Au17	Au16	Ag16	122.6 (4)	Au16	Au17	Ag10	114.2 (3)	Ag12	Au18	Ag14	56.3 (4)
Au4	Au15	Au14	174.5 (3)	Au17	Au16	Ag17	59.6 (3)	Au16	Au17	Ag17	59.6 (3)	Ag12	Au18	Ag17	159.9 (5)
Au4	Au15	Au16	117.0 (3)	Au17	Au16	Ag18	57.0 (3)	Au16	Au17	Ag18	64.4 (3)	Ag12	Au18	Ag18	84.4 (4)
Au4	Au15	Ag3	119.1 (4)	Au18	Au16	Ag5	143.1 (4)	Au18	Au17	Ag7	114.7 (3)	Ag13	Au18	Ag14	107.8 (4)
Au4	Au15	Ag4	123.6 (4)	Au18	Au16	Ag6	155.2 (4)	Au18	Au17	Ag8	109.8 (3)	Ag13	Au18	Ag17	65.7 (3)
Au4	Au15	Ag5	65.6 (3)	Au18	Au16	Ag7	112.1 (4)	Au18	Au17	Ag9	62.2 (3)	Ag13	Au18	Ag18	159.9 (5)
Au4	Au15	Ag6	64.7 (3)	Au18	Au16	Ag8	106.1 (4)	Au18	Au17	Ag10	61.1 (3)	Ag14	Au18	Ag17	143.1 (5)
Au4	Au15	Ag15	114.2 (4)	Au18	Au16	Ag15	90.6 (3)	Au18	Au17	Ag17	65.8 (3)	Ag14	Au18	Ag18	65.2 (3)
Au4	Au15	Ag16	117.7 (3)	Au18	Au16	Ag16	95.5 (4)	Au18	Au17	Ag18	59.8 (3)	Ag17	Au18	Ag18	107.8 (4)

Table III (Continued)

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
Au2	Ag1	Au7	57.0 (3)	Au14	Ag3	Cl1	104 (1)	Ag15	Ag5	C17	52.9 (7)	Au17	Ag8	Ag18	59.4 (3)
Au2	Ag1	Au13	56.5 (3)	Au15	Ag3	Ag1	117.9 (5)	C15	Ag5	C17	84 (1)	Au17	Ag8	C16	153 (1)
Au2	Ag1	Au14	107.7 (4)	Au15	Ag3	Ag4	59.0 (3)	Au4	Ag6	Au10	60.4 (3)	Au17	Ag8	C18	112.4 (7)
Au2	Ag1	Ag2	60.7 (4)	Au15	Ag3	Ag15	58.9 (3)	Au4	Ag6	Au15	57.3 (3)	Ag6	Ag8	Ag7	79.9 (4)
Au2	Ag1	Ag3	138.8 (4)	Au15	Ag3	Cl1	164 (1)	Au4	Ag6	Au16	109.9 (3)	Ag6	Ag8	Ag18	97.9 (4)
Au2	Ag1	Ag13	106.0 (5)	Ag1	Ag3	Ag4	97.4 (5)	Au4	Ag6	Ag5	61.5 (4)	Ag6	Ag8	C16	50.0 (8)
Au2	Ag1	Cl1	117 (1)	Ag1	Ag3	Ag15	82.1 (4)	Au4	Ag6	Ag8	158.1 (5)	Ag6	Ag8	C18	71.6 (9)
Au2	Ag1	C13	148.7 (9)	Ag1	Ag3	Cl1	47 (1)	Au4	Ag6	Ag16	108.3 (4)	Ag7	Ag8	Ag18	109.8 (4)
Au7	Ag1	Au13	54.6 (3)	Ag4	Ag3	Ag15	107.8 (5)	Au4	Ag6	C16	134 (1)	Ag7	Ag8	C16	95 (1)
Au7	Ag1	Au14	106.4 (4)	Ag4	Ag3	Cl1	114 (1)	Au10	Ag6	Au15	56.3 (2)	Ag7	Ag8	C18	142.7 (7)
Au7	Ag1	Ag2	105.2 (5)	Ag15	Ag3	Cl1	116 (1)	Au10	Ag6	Au16	106.4 (3)	Ag18	Ag8	C16	135.9 (9)
Au7	Ag1	Ag3	156.2 (4)	Au3	Ag4	Au10	57.0 (3)	Au10	Ag6	Ag5	108.1 (4)	Ag18	Ag8	C18	53.2 (8)
Au7	Ag1	Ag13	57.6 (3)	Au3	Ag4	Au14	108.5 (4)	Au10	Ag6	Ag8	137.5 (5)	C16	Ag8	C18	85 (1)
Au7	Ag1	Cl1	148 (1)	Au3	Ag4	Au15	57.0 (3)	Au10	Ag6	Ag16	59.0 (3)	Au6	Ag9	Au11	58.7 (2)
Au7	Ag1	C13	92.2 (8)	Au3	Ag4	Ag2	139.2 (4)	Au10	Ag6	C16	135.8 (9)	Au6	Ag9	Au17	57.7 (3)
Au13	Ag1	Au14	59.6 (3)	Au3	Ag4	Ag3	60.9 (4)	Au15	Ag6	Au16	60.5 (2)	Au6	Ag9	Au18	108.2 (4)
Au13	Ag1	Ag2	58.6 (4)	Au3	Ag4	Ag16	106.5 (4)	Au15	Ag6	Ag5	58.3 (3)	Au6	Ag9	Ag10	59.9 (3)
Au13	Ag1	Ag3	114.4 (4)	Au3	Ag4	Cl2	117 (1)	Au15	Ag6	Ag8	117.5 (4)	Au6	Ag9	Ag11	133.7 (6)
Au13	Ag1	Ag13	59.6 (3)	Au3	Ag4	Cl4	146.6 (7)	Au15	Ag6	Ag16	59.0 (3)	Au6	Ag9	Ag17	109.0 (4)
Au13	Ag1	Cl1	153 (1)	Au10	Ag4	Au14	107.4 (4)	Au15	Ag6	C16	165 (1)	Au6	Ag9	C19	109 (1)
Au13	Ag1	C13	112.6 (8)	Au10	Ag4	Au15	54.6 (2)	Au16	Ag6	Ag5	60.6 (3)	Au6	Ag9	C111	150.4 (7)
Au14	Ag1	Ag2	59.5 (3)	Au10	Ag4	Ag2	158.1 (5)	Au16	Ag6	Ag8	57.7 (3)	Au11	Ag9	Au17	56.0 (2)
Au14	Ag1	Ag3	55.7 (3)	Au10	Ag4	Ag3	105.5 (5)	Au16	Ag6	Ag16	58.4 (4)	Au11	Ag9	Au18	109.3 (5)
Au14	Ag1	Ag13	63.5 (3)	Au10	Ag4	Ag16	57.9 (3)	Au16	Ag6	C16	104 (1)	Au11	Ag9	Ag10	106.7 (4)
Au14	Ag1	Cl1	105 (1)	Au10	Ag4	Cl2	146.2 (9)	Ag5	Ag6	Ag8	97.2 (4)	Au11	Ag9	Ag11	162.2 (6)
Au14	Ag1	C13	84.9 (6)	Au10	Ag4	Cl4	90.6 (6)	Ag5	Ag6	Ag16	106.9 (4)	Au11	Ag9	Ag17	59.3 (3)
Ag2	Ag1	Ag3	80.2 (4)	Au14	Ag4	Au15	60.3 (3)	Ag5	Ag6	C16	114.5 (9)	Au11	Ag9	C19	144 (1)
Ag2	Ag1	Ag13	110.2 (5)	Au14	Ag4	Ag2	57.2 (3)	Ag8	Ag6	Ag16	81.5 (4)	Au11	Ag9	C111	92.8 (7)
Ag2	Ag1	Cl1	95 (1)	Au14	Ag4	Ag3	59.8 (4)	Ag8	Ag6	C16	48 (1)	Au17	Ag9	Au18	60.5 (3)
Ag2	Ag1	C13	143.4 (7)	Au14	Ag4	Ag16	64.3 (4)	Ag16	Ag6	C16	116 (1)	Au17	Ag9	Ag10	59.4 (4)
Ag3	Ag1	Ag13	98.6 (4)	Au14	Ag4	Cl2	105.7 (9)	Au5	Ag7	Au11	60.4 (3)	Au17	Ag9	Ag11	116.2 (4)
Ag3	Ag1	Cl1	51.1 (9)	Au14	Ag4	Cl4	87.1 (7)	Au5	Ag7	Au16	109.7 (5)	Au17	Ag9	Ag17	60.9 (3)
Ag3	Ag1	C13	72.0 (8)	Au15	Ag4	Ag2	116.6 (5)	Au5	Ag7	Au17	57.1 (3)	Au17	Ag9	C19	151 (1)
Ag13	Ag1	Cl1	137 (1)	Au15	Ag4	Ag3	59.2 (3)	Au5	Ag7	Ag5	160.4 (4)	Au17	Ag9	C111	115.5 (9)
Ag13	Ag1	C13	53.3 (8)	Au15	Ag4	Ag16	59.7 (3)	Au5	Ag7	Ag8	61.1 (4)	Au18	Ag9	Ag10	59.4 (4)
Cl1	Ag1	C13	86 (1)	Au15	Ag4	Cl2	155.4 (9)	Au5	Ag7	Ag17	108.8 (5)	Au18	Ag9	Ag11	57.4 (3)
Au2	Ag2	Au8	60.1 (3)	Au15	Ag4	Cl4	112.7 (6)	Au5	Ag7	C15	132.6 (8)	Au18	Ag9	Ag17	65.1 (4)
Au2	Ag2	Au13	57.3 (3)	Ag2	Ag4	Ag3	81.1 (4)	Au11	Ag7	Au16	107.1 (4)	Au18	Ag9	C19	107 (1)
Au2	Ag2	Au14	110.7 (5)	Ag2	Ag4	Ag16	100.2 (5)	Au11	Ag7	Au17	57.1 (3)	Au18	Ag9	C111	88.0 (8)
Au2	Ag2	Ag1	61.9 (4)	Ag2	Ag4	Cl2	49.6 (9)	Au11	Ag7	Ag5	135.1 (4)	Ag10	Ag9	Ag11	77.6 (4)
Au2	Ag2	Ag4	161.1 (5)	Ag2	Ag4	Cl4	74.1 (7)	Au11	Ag7	Ag8	109.1 (5)	Ag10	Ag9	Ag17	112.1 (5)
Au2	Ag2	Ag14	108.2 (5)	Ag3	Ag4	Ag16	111.1 (5)	Au11	Ag7	Ag17	60.0 (3)	Ag10	Ag9	C19	92 (1)
Au2	Ag2	Cl2	132.1 (7)	Ag3	Ag4	Cl2	96.5 (8)	Au11	Ag7	C15	129 (1)	Ag10	Ag9	C111	145.8 (8)
Au8	Ag2	Au13	56.8 (3)	Ag3	Ag4	Cl4	146.1 (8)	Au16	Ag7	Au17	60.4 (3)	Ag11	Ag9	Ag17	103.0 (5)
Au8	Ag2	Au14	107.0 (5)	Ag16	Ag4	Cl2	136 (1)	Au16	Ag7	Ag5	57.9 (3)	Ag11	Ag9	C19	51.2 (8)
Au8	Ag2	Ag1	109.6 (5)	Ag16	Ag4	Cl4	53.1 (6)	Au16	Ag7	Ag8	61.5 (3)	Ag11	Ag9	C111	75.9 (7)
Au8	Ag2	Ag4	135.0 (4)	Cl2	Ag4	Cl4	85 (1)	Au16	Ag7	Ag17	58.5 (3)	Ag17	Ag9	C19	141 (1)
Au8	Ag2	Ag14	59.2 (3)	Au4	Ag5	Au9	57.1 (3)	Au16	Ag7	C15	109.5 (9)	Ag17	Ag9	C111	54.8 (8)
Au8	Ag2	Cl2	130 (1)	Au4	Ag5	Au15	57.2 (3)	Au17	Ag7	Ag5	117.0 (4)	C19	Ag9	C111	88 (1)
Au13	Ag2	Au14	60.9 (4)	Au4	Ag5	Au16	108.6 (4)	Au17	Ag7	Ag8	59.2 (4)	Au6	Ag10	Au12	60.8 (3)
Au13	Ag2	Ag1	59.9 (4)	Au4	Ag5	Ag6	60.7 (4)	Au17	Ag7	Ag17	59.6 (3)	Au6	Ag10	Au17	57.6 (3)
Au13	Ag2	Ag4	117.4 (4)	Au4	Ag5	Ag7	138.9 (4)	Au17	Ag7	C15	169.6 (9)	Au6	Ag10	Au18	109.8 (4)
Au13	Ag2	Ag14	59.4 (3)	Au4	Ag5	Ag15	107.1 (4)	Ag5	Ag7	Ag8	99.5 (5)	Au6	Ag10	Ag9	61.1 (3)
Au13	Ag2	Cl2	169.4 (8)	Au4	Ag5	C15	117 (1)	Ag5	Ag7	Ag17	78.7 (4)	Au6	Ag10	Ag12	160.8 (5)
Au14	Ag2	Ag1	62.2 (3)	Au4	Ag5	C17	146.7 (8)	Ag5	Ag7	C15	52.6 (8)	Au6	Ag10	Ag18	108.3 (5)
Au14	Ag2	Ag4	57.7 (3)	Au9	Ag5	Au15	55.0 (3)	Ag8	Ag7	Ag17	108.6 (5)	Au6	Ag10	C110	134 (1)
Au14	Ag2	Ag14	58.6 (3)	Au9	Ag5	Au16	108.1 (4)	Ag8	Ag7	C15	120 (1)	Au12	Ag10	Au17	56.3 (3)
Au14	Ag2	Cl2	108.6 (9)	Au9	Ag5	Ag6	105.6 (4)	Ag17	Ag7	C15	114.0 (9)	Au12	Ag10	Au18	106.2 (5)
Ag1	Ag2	Ag4	99.4 (5)	Au9	Ag5	Ag7	158.8 (5)	Au5	Ag8	Au12	57.8 (4)	Au12	Ag10	Ag9	107.5 (4)
Ag1	Ag2	Ag14	109.1 (4)	Au9	Ag5	Ag15	58.1 (3)	Au5	Ag8	Au16	107.8 (4)	Au12	Ag10	Ag12	134.4 (5)
Ag1	Ag2	Cl2	118 (1)	Au9	Ag5	C15	145 (1)	Au5	Ag8	Au17	56.9 (3)	Au12	Ag10	Ag18	59.1 (3)
Ag4	Ag2	Ag14	79.3 (3)	Au9	Ag5	C17	90.7 (7)	Au5	Ag8	Ag6	138.4 (5)	Au12	Ag10	C110	129.5 (9)
Ag4	Ag2	Cl2	52.0 (7)	Au15	Ag5	Au16	60.5 (3)	Au5	Ag8	Ag7	60.6 (4)	Au17	Ag10	Au18	60.2 (3)
Ag14	Ag2	Cl2	115.2 (8)	Au15	Ag5	Ag6	59.1 (3)	Au5	Ag8	Ag18	107.0 (5)	Au17	Ag10	Ag9	57.6 (4)
Au3	Ag3	Au9	60.3 (4)	Au15	Ag5	Ag7	116.9 (5)	Au5	Ag8	C16	117.0 (9)	Au17	Ag10	Ag12	117.1 (5)
Au3	Ag3	Au14	109.5 (4)	Au15	Ag5	Ag15	60.4 (3)	Au5	Ag8	C18	150 (1)	Au17	Ag10	Ag18	58.3 (4)
Au3	Ag3	Au15	57.1 (2)	Au15	Ag5	C15	157 (1)	Au12	Ag8	Au16	106.6 (4)	Au17	Ag10	C110	168 (1)
Au3	Ag3	Ag1	158.2 (6)	Au15	Ag5	C17	113.2 (7)	Au12	Ag8	Au17	54.9 (3)	Au18	Ag10	Ag9	60.1 (4)
Au3	Ag3	Ag4	61.3 (4)	Au16	Ag5	Ag6	59.7 (4)	Au12	Ag8	Ag6	156.3 (4)	Au18	Ag10	Ag12	58.3 (4)
Au3	Ag3	Ag15	107.9 (4)	Au16	Ag5	Ag7	57.3 (3)	Au12	Ag8	Ag7	105.8 (5)	Au18	Ag10	Ag18	57.9 (4)
Au3	Ag3	Cl1	134 (1)	Au16	Ag5	Ag15	65.3 (4)	Au12	Ag8	Ag18	58.5 (4)	Au18	Ag10	C110	108.1 (9)
Au9	Ag3	Au14	106.6 (4)	Au16	Ag5	C15	106 (1)	Au12	Ag8	C16	148.3 (9)	Ag9	Ag10	Ag12	100.0 (4)
Au9	Ag3	Au15	56.2 (3)	Au16	Ag5	C17	87.8 (9)	Au12	Ag8	C18	92.4 (9)	Ag9	Ag10	Ag18	105.6 (6)
Au9	Ag3	Ag1	137.7 (5)	Ag6	Ag5	Ag7	81.2 (4)	Au16	Ag8	Au17	59.6 (3)	Ag9	Ag10	C110	121.5 (9)
Au9	Ag3	Ag4	108.4 (5)	Ag6	Ag5	Ag15	111.9 (5)	Au16	Ag8	Ag6	55.8 (3)	Ag12	Ag10	Ag18	79.0 (4)
Au9	Ag3	Ag15	58.7 (3)	Ag6	Ag5	C15	97.9 (9)	Au16	Ag8	Ag7	59.6 (3)	Ag12	Ag10	C110	50.7 (9)
Au9	Ag3	Cl1	136 (1)	Ag6	Ag5	C17	147 (1)	Au16	Ag8	Ag18	62.5 (3)	Ag18	Ag10	C110	113 (1)
Au14	Ag3	Au15	60.5 (3)	Ag7	Ag5	Ag15	100.6 (5)	Au16	Ag8	C16	104.5 (9)	Au1	Ag11	Au7	61.0 (2)
Au14	Ag3	Ag1	58.2 (4)	Ag7	Ag5	C15	50 (1)	Au16	Ag8	C18	84.3 (7)	Au1	Ag11	Au13	57.9 (3)
Au14	Ag3	Ag4	60.6 (4)	Ag7	Ag5	C17	74.4 (8)	Au17	Ag8	Ag6	114.5 (4)	Au1	Ag11	Au18	110.2 (5)
Au14	Ag3	Ag15	59.2 (4)	Ag15	Ag5	C15	135 (1)	Au17	Ag8	Ag7	58.9 (3)	Au1	Ag11	Ag9	160.6 (4)

Table III (Continued)

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
Au1	Ag11	Ag12	60.7 (3)	Au14	Ag13	Ag17	82.9 (3)	Au14	Ag15	Ag5	107.3 (4)	Au11	Ag17	Ag7	60.1 (3)
Au1	Ag11	Ag13	108.9 (4)	Au14	Ag13	Cl3	91.3 (9)	Au14	Ag15	Ag13	59.9 (4)	Au11	Ag17	Ag9	63.7 (3)
Au1	Ag11	Cl9	133 (1)	Au14	Ag13	Cl11	136.9 (8)	Au14	Ag15	Ag17	88.7 (4)	Au11	Ag17	Ag13	140.7 (5)
Au7	Ag11	Au13	56.5 (3)	Au18	Ag13	Ag1	108.1 (4)	Au14	Ag15	Cl3	98.0 (9)	Au11	Ag17	Ag15	157.5 (5)
Au7	Ag11	Au18	106.9 (5)	Au18	Ag13	Ag11	59.9 (4)	Au14	Ag15	Cl7	141 (1)	Au11	Ag17	Cl7	110.1 (8)
Au7	Ag11	Ag9	134.4 (5)	Au18	Ag13	Ag15	87.0 (4)	Au15	Ag15	Au16	57.7 (3)	Au11	Ag17	Cl11	103.1 (9)
Au7	Ag11	Ag12	107.5 (4)	Au18	Ag13	Ag17	60.5 (3)	Au15	Ag15	Ag3	58.3 (3)	Au16	Ag17	Au17	60.7 (3)
Au7	Ag11	Ag13	58.9 (3)	Au18	Ag13	Cl3	138.4 (9)	Au15	Ag15	Ag5	58.7 (3)	Au16	Ag17	Au18	56.9 (3)
Au7	Ag11	Cl9	131.8 (9)	Au18	Ag13	Cl11	98.8 (8)	Au15	Ag15	Ag13	120.0 (5)	Au16	Ag17	Ag7	60.8 (3)
Au13	Ag11	Au18	60.6 (3)	Ag1	Ag13	Ag11	111.5 (5)	Au15	Ag15	Ag17	111.5 (4)	Au16	Ag17	Ag9	106.9 (5)
Au13	Ag11	Ag9	116.8 (5)	Ag1	Ag13	Ag15	81.9 (4)	Au15	Ag15	Cl3	142.5 (9)	Au16	Ag17	Ag13	89.5 (4)
Au13	Ag11	Ag12	57.7 (4)	Ag1	Ag13	Ag17	136.7 (5)	Au15	Ag15	Cl7	129.5 (8)	Au16	Ag17	Ag15	62.9 (4)
Au13	Ag11	Ag13	59.1 (4)	Ag1	Ag13	Cl3	69.3 (8)	Au16	Ag15	Ag3	104.8 (5)	Au16	Ag17	Cl7	104 (1)
Au13	Ag11	Cl9	167.4 (9)	Ag1	Ag13	Cl11	152 (1)	Au16	Ag15	Ag5	58.7 (4)	Au16	Ag17	Cl11	139.4 (8)
Au18	Ag11	Ag9	57.6 (3)	Ag11	Ag13	Ag15	146.5 (4)	Au16	Ag15	Ag13	84.6 (4)	Au17	Ag17	Au18	57.4 (3)
Au18	Ag11	Ag12	60.6 (4)	Ag11	Ag13	Ag17	98.1 (4)	Au16	Ag15	Ag17	54.3 (3)	Au17	Ag17	Ag7	58.3 (3)
Au18	Ag11	Ag13	59.1 (4)	Ag11	Ag13	Cl3	161.5 (9)	Au16	Ag15	Cl3	139 (1)	Au17	Ag17	Ag9	58.2 (3)
Au18	Ag11	Cl9	106.9 (9)	Ag11	Ag13	Cl11	87 (1)	Au16	Ag15	Cl7	93.9 (8)	Au17	Ag17	Ag13	110.4 (4)
Ag9	Ag11	Ag12	100.2 (4)	Ag15	Ag13	Ag17	57.1 (3)	Ag3	Ag15	Ag5	111.4 (5)	Au17	Ag17	Ag15	123.1 (4)
Ag9	Ag11	Ag13	78.8 (4)	Ag15	Ag13	Cl3	51.4 (8)	Ag3	Ag15	Ag13	96.1 (4)	Au17	Ag17	Cl7	147.0 (9)
Ag9	Ag11	Cl9	51 (1)	Ag15	Ag13	Cl11	94 (1)	Ag3	Ag15	Ag17	148.1 (6)	Au17	Ag17	Cl11	124 (1)
Ag12	Ag11	Ag13	107.0 (5)	Ag17	Ag13	Cl3	92.2 (7)	Ag3	Ag15	Cl3	84.5 (8)	Au18	Ag17	Ag7	105.0 (5)
Ag12	Ag11	Cl9	119 (1)	Ag17	Ag13	Cl11	54.2 (8)	Ag3	Ag15	Cl7	159 (1)	Au18	Ag17	Ag9	58.4 (4)
Ag13	Ag11	Cl9	115 (1)	Cl3	Ag13	Cl11	87 (1)	Ag5	Ag15	Ag13	138.0 (5)	Au18	Ag17	Ag13	53.9 (3)
Au1	Ag12	Au8	58.8 (3)	Au8	Ag14	Au13	56.6 (2)	Ag5	Ag15	Ag17	80.0 (4)	Au18	Ag17	Ag15	86.0 (4)
Au1	Ag12	Au13	58.4 (3)	Au8	Ag14	Au14	109.0 (4)	Ag5	Ag15	Cl3	154 (1)	Au18	Ag17	Cl7	141.9 (9)
Au1	Ag12	Au18	109.4 (5)	Au8	Ag14	Au18	107.9 (4)	Ag5	Ag15	Cl7	70.9 (8)	Au18	Ag17	Cl11	90.5 (9)
Au1	Ag12	Ag10	134.6 (5)	Au8	Ag14	Ag2	60.2 (3)	Ag13	Ag15	Ag17	61.1 (3)	Ag7	Ag17	Ag9	110.5 (5)
Au1	Ag12	Ag11	60.7 (3)	Au8	Ag14	Ag12	63.6 (3)	Ag13	Ag15	Cl3	54 (1)	Ag7	Ag17	Ag13	150.2 (5)
Au1	Ag12	Ag14	109.3 (5)	Au8	Ag14	Ag16	157.2 (5)	Ag13	Ag15	Cl7	94 (1)	Ag7	Ag17	Ag15	99.6 (5)
Au1	Ag12	Cl10	112.2 (9)	Au8	Ag14	Ag18	141.9 (5)	Ag17	Ag15	Cl3	97 (1)	Ag7	Ag17	Cl7	88.8 (9)
Au1	Ag12	Cl12	151.0 (7)	Au8	Ag14	Cl4	110.2 (7)	Ag17	Ag15	Cl7	52 (1)	Ag7	Ag17	Cl11	159.7 (8)
Au8	Ag12	Au13	55.9 (3)	Au8	Ag14	Cl12	105.7 (8)	Cl3	Ag15	Cl7	87 (1)	Ag9	Ag17	Ag13	78.0 (4)
Au8	Ag12	Au18	109.2 (5)	Au13	Ag14	Au14	60.8 (3)	Au10	Ag16	Au14	107.7 (4)	Ag9	Ag17	Ag15	137.7 (4)
Au8	Ag12	Ag10	161.4 (6)	Au13	Ag14	Au18	57.8 (3)	Au10	Ag16	Au15	56.4 (3)	Ag9	Ag17	Cl7	149 (1)
Au8	Ag12	Ag11	106.8 (5)	Au13	Ag14	Ag2	57.5 (3)	Au10	Ag16	Au16	108.6 (5)	Ag9	Ag17	Cl11	66 (1)
Au8	Ag12	Ag14	59.0 (3)	Au13	Ag14	Ag12	58.0 (3)	Au10	Ag16	Ag4	64.1 (4)	Ag13	Ag17	Ag15	61.7 (3)
Au8	Ag12	Cl10	143.8 (9)	Au13	Ag14	Ag16	122.0 (5)	Au10	Ag16	Ag6	60.0 (4)	Ag13	Ag17	Cl7	97.7 (8)
Au8	Ag12	Cl12	93.4 (7)	Au13	Ag14	Ag18	110.6 (4)	Au10	Ag16	Ag14	143.5 (4)	Ag13	Ag17	Cl11	50.1 (7)
Au13	Ag12	Au18	60.8 (3)	Au13	Ag14	Cl4	144.7 (8)	Au10	Ag16	Ag18	155.7 (4)	Ag15	Ag17	Cl7	56.4 (9)
Au13	Ag12	Ag10	116.1 (5)	Au13	Ag14	Cl12	126.3 (9)	Au10	Ag16	Cl4	104.8 (9)	Ag15	Ag17	Cl11	94.3 (9)
Au13	Ag12	Ag11	59.5 (4)	Au14	Ag14	Au18	56.9 (3)	Au10	Ag16	Cl8	111 (1)	Cl7	Ag17	Cl11	87 (1)
Au13	Ag12	Ag14	60.8 (4)	Au14	Ag14	Ag2	60.0 (4)	Au14	Ag16	Au15	58.0 (3)	Au12	Ag18	Au16	108.9 (4)
Au13	Ag12	Cl10	154 (1)	Au14	Ag14	Ag12	106.9 (5)	Au14	Ag16	Au16	57.8 (3)	Au12	Ag18	Au17	56.6 (3)
Au13	Ag12	Cl12	114.6 (8)	Au14	Ag14	Ag16	61.8 (4)	Au14	Ag16	Ag4	58.5 (3)	Au12	Ag18	Au18	108.3 (4)
Au18	Ag12	Ag10	57.0 (4)	Au14	Ag14	Ag18	88.5 (4)	Au14	Ag16	Ag6	105.5 (4)	Au12	Ag18	Ag8	63.9 (3)
Au18	Ag12	Ag11	59.6 (4)	Au14	Ag14	Cl4	102 (1)	Au14	Ag16	Ag14	54.8 (3)	Au12	Ag18	Ag10	59.9 (3)
Au18	Ag12	Ag14	64.9 (4)	Au14	Ag14	Cl12	137.9 (8)	Au14	Ag16	Ag18	84.7 (3)	Au12	Ag18	Ag14	155.8 (5)
Au18	Ag12	Cl10	106.8 (9)	Au18	Ag14	Ag2	104.3 (4)	Au14	Ag16	Cl4	92.8 (7)	Au12	Ag18	Ag16	145.6 (4)
Au18	Ag12	Cl12	85.9 (8)	Au18	Ag14	Ag12	58.8 (4)	Au14	Ag16	Cl8	139 (1)	Au12	Ag18	Cl8	105.8 (8)
Ag10	Ag12	Ag11	77.9 (4)	Au18	Ag14	Ag16	84.9 (4)	Au15	Ag16	Au16	60.9 (4)	Au12	Ag18	Cl12	110.1 (9)
Ag10	Ag12	Ag14	102.4 (5)	Au18	Ag14	Ag18	53.4 (3)	Au15	Ag16	Ag4	58.8 (3)	Au16	Ag18	Au17	58.7 (3)
Ag10	Ag12	Cl10	50.7 (9)	Au18	Ag14	Cl4	140.9 (8)	Au15	Ag16	Ag6	58.2 (3)	Au16	Ag18	Au18	57.7 (3)
Ag10	Ag12	Cl12	74.4 (6)	Au18	Ag14	Cl12	90.3 (7)	Au15	Ag16	Ag14	112.3 (4)	Au16	Ag18	Ag8	60.1 (4)
Ag11	Ag12	Ag14	112.0 (6)	Ag2	Ag14	Ag12	109.9 (4)	Au15	Ag16	Ag18	120.2 (5)	Au16	Ag18	Ag10	105.6 (5)
Ag11	Ag12	Cl10	94.7 (9)	Ag2	Ag14	Ag16	98.9 (5)	Au15	Ag16	Cl4	128.1 (7)	Au16	Ag18	Ag14	84.6 (3)
Ag11	Ag12	Cl12	144.0 (8)	Ag2	Ag14	Ag18	148.4 (5)	Au15	Ag16	Cl8	141.8 (9)	Au16	Ag18	Ag16	54.2 (4)
Ag14	Ag12	Cl10	137.9 (9)	Ag2	Ag14	Cl4	87.3 (8)	Au16	Ag16	Ag4	107.7 (4)	Au16	Ag18	Cl8	91 (1)
Ag14	Ag12	Cl12	54.1 (8)	Ag2	Ag14	Cl12	162.1 (8)	Au16	Ag16	Ag6	60.2 (4)	Au16	Ag18	Cl12	140.0 (9)
Cl10	Ag12	Cl12	85 (1)	Ag12	Ag14	Ag16	137.7 (4)	Au16	Ag16	Ag14	89.1 (4)	Au17	Ag18	Au18	60.8 (3)
Au7	Ag13	Au13	56.7 (3)	Ag12	Ag14	Ag18	79.2 (4)	Au16	Ag16	Ag18	59.8 (4)	Au17	Ag18	Ag8	59.1 (4)
Au7	Ag13	Au14	108.7 (4)	Ag12	Ag14	Cl4	151 (1)	Au16	Ag16	Cl4	140.7 (9)	Au17	Ag18	Ag10	58.2 (3)
Au7	Ag13	Au18	108.4 (4)	Ag12	Ag14	Cl12	68.7 (9)	Au16	Ag16	Cl8	97.3 (9)	Au17	Ag18	Ag14	121.7 (4)
Au7	Ag13	Ag1	64.3 (3)	Ag16	Ag14	Ag18	60.8 (3)	Ag4	Ag16	Ag6	111.2 (5)	Au17	Ag18	Ag16	112.5 (5)
Au7	Ag13	Ag11	60.0 (3)	Ag16	Ag14	Cl4	56.2 (8)	Ag4	Ag16	Ag14	80.3 (4)	Au17	Ag18	Cl8	127.2 (9)
Au7	Ag13	Ag15	145.7 (4)	Ag16	Ag14	Cl12	92.6 (8)	Ag4	Ag16	Ag18	137.9 (5)	Au17	Ag18	Cl12	145 (1)
Au7	Ag13	Ag17	156.9 (5)	Ag18	Ag14	Cl4	98.4 (7)	Ag4	Ag16	Cl4	69.5 (8)	Au18	Ag18	Ag8	108.6 (5)
Au7	Ag13	Cl3	107.0 (7)	Ag18	Ag14	Cl12	49.5 (7)	Ag4	Ag16	Cl8	154.7 (9)	Au18	Ag18	Ag10	59.6 (4)
Au7	Ag13	Cl11	113 (1)	Cl4	Ag14	Cl12	88 (1)	Ag6	Ag16	Ag14	149.1 (5)	Au18	Ag18	Ag14	61.4 (3)
Au13	Ag13	Au14	58.2 (3)	Au9	Ag15	Au14	108.2 (4)	Ag6	Ag16	Ag18	96.9 (5)	Au18	Ag18	Ag16	88.1 (4)
Au13	Ag13	Au18	60.6 (3)	Au9	Ag15	Au15	56.6 (3)	Ag6	Ag16	Cl4	159.0 (9)	Au18	Ag18	Cl8	140 (1)
Au13	Ag13	Ag1	59.1 (3)	Au9	Ag15	Au16	108.0 (4)	Ag6	Ag16	Cl8	84.0 (9)	Au18	Ag18	Cl12	101.4 (8)
Au13	Ag13	Ag11	58.3 (3)	Au9	Ag15	Ag3	60.2 (4)	Ag14	Ag16	Ag18	60.7 (3)	Ag8	Ag18	Ag10	111.1 (5)
Au13	Ag13	Ag15	111.8 (4)	Au9	Ag15	Ag5	64.5 (4)	Ag14	Ag16	Cl4	51.5 (8)	Ag8	Ag18	Ag14	138.8 (6)
Au13	Ag13	Ag17	120.4 (4)	Au9	Ag15	Ag13	155.0 (4)	Ag14	Ag16	Cl8	97 (1)	Ag8	Ag18	Ag16	82.5 (4)
Au13	Ag13	Cl3	128.0 (8)	Au9	Ag15	Ag17	143.7 (4)	Ag18	Ag16	Cl4	95.1 (9)	Ag8	Ag18	Cl8	68.5 (8)
Au13	Ag13	Cl11	145 (1)	Au9	Ag15	Cl3	111 (1)	Ag18	Ag16	Cl8	54 (1)	Ag8	Ag18	Cl12	149.8 (8)
Au14	Ag13	Au18	57.0 (3)	Au9	Ag15	Cl7	106 (1)	Cl4	Ag16	Cl8	89 (1)	Ag10	Ag18	Ag14	97.8 (4)
Au14	Ag13	Ag1	59.8 (3)	Au14	Ag15	Au15	60.4 (3)	Au11	Ag17	Au16	109.1 (4)	Ag10	Ag18	Ag16	147.3 (4)
Au14	Ag13	Ag11	105.1 (4)	Au14	Ag15	Au16	57.1 (3)	Au11	Ag17	Au17	56.8 (3)	Ag10	Ag18	Cl8	161 (1)
Au14	Ag13	Ag15	53.9 (4)	Au14	Ag15	Ag3	59.6 (4)	Au11	Ag17	Au18	107.6 (4)	Ag10	Ag18	Cl12	87 (1)

Table III (Continued)

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
Ag14	Ag18	Ag16	58.5 (3)	Cl12	Ag20	Cl14	123 (2)	Ag5	Cl7	Ag15	56.2 (7)	Ag9	Cl11	Ag19	148 (1)
Ag14	Ag18	Cl8	93.5 (8)	Ag1	Cl1	Ag3	82 (1)	Ag5	Cl7	Ag17	82 (1)	Ag13	Cl11	Ag17	76 (1)
Ag14	Ag18	Cl12	55.8 (8)	Ag2	Cl2	Ag4	78 (1)	Ag5	Cl7	Ag19	144 (1)	Ag13	Cl11	Ag19	93 (1)
Ag16	Ag18	Cl8	51.6 (9)	Ag1	Cl3	Ag13	57.4 (8)	Ag15	Cl7	Ag17	72 (1)	Ag17	Cl11	Ag19	90 (1)
Ag16	Ag18	Cl12	95 (1)	Ag1	Cl3	Ag15	87 (1)	Ag15	Cl7	Ag19	89 (1)	Ag12	Cl12	Ag14	57.2 (7)
Cl8	Ag18	Cl12	86 (1)	Ag1	Cl3	Ag19	148 (2)	Ag17	Cl7	Ag19	94 (1)	Ag12	Cl12	Ag18	85 (1)
Cl3	Ag19	Cl7	92 (1)	Ag13	Cl3	Ag15	74 (1)	Ag8	Cl8	Ag16	88 (1)	Ag12	Cl12	Ag20	146 (1)
Cl3	Ag19	Cl11	89 (1)	Ag13	Cl3	Ag19	91 (1)	Ag8	Cl8	Ag18	58.3 (7)	Ag14	Cl12	Ag18	75 (1)
Cl3	Ag19	Cl13	128 (1)	Ag15	Cl3	Ag19	92 (1)	Ag8	Cl8	Ag20	149 (2)	Ag14	Cl12	Ag20	90 (1)
Cl7	Ag19	Cl11	87 (1)	Ag4	Cl4	Ag14	83.7 (9)	Ag16	Cl8	Ag18	74 (1)	Ag18	Cl12	Ag20	94 (1)
Cl7	Ag19	Cl13	126 (1)	Ag4	Cl4	Ag16	57.5 (7)	Ag16	Cl8	Ag20	92 (1)	Ag13	Ag19	Ag15	51.5 (3)
Cl11	Ag19	Cl13	123 (2)	Ag4	Cl4	Ag20	143 (1)	Ag18	Cl8	Ag20	92 (1)	Ag13	Ag19	Ag17	50.5 (3)
Cl4	Ag20	Cl8	92 (1)	Ag14	Cl4	Ag16	72.3 (8)	Ag9	Cl9	Ag11	78 (1)	Ag15	Ag19	Ag17	48.8 (3)
Cl4	Ag20	Cl12	87 (1)	Ag14	Cl4	Ag20	93 (1)	Ag10	Cl10	Ag12	79 (1)	Ag14	Ag20	Ag16	49.0 (3)
Cl4	Ag20	Cl14	125 (1)	Ag16	Cl4	Ag20	86.8 (8)	Ag9	Cl11	Ag13	86 (1)	Ag14	Ag20	Ag18	49.8 (3)
Cl8	Ag20	Cl12	87 (1)	Ag5	Cl5	Ag7	78 (1)	Ag9	Cl11	Ag17	58.8 (8)	Ag16	Ag20	Ag18	50.6 (3)
Cl8	Ag20	Cl14	130 (1)	Ag6	Cl6	Ag8	82.3 (9)								

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

the apical Ag atoms are best considered as nonbonding.

The terminal, doubly, and triply bridging Ag–Cl distances fall in the range of 2.37–2.38, 2.35–2.53, and 2.51–2.73 Å, with an average of 2.37, 2.44, and 2.62 Å, respectively. The 12 Au–P distances fall in the range of 2.29–2.47 Å, with an average of 2.38 Å.

C. 13-Atom Icosahedral Cluster Units. The basic building block of the 38-atom cluster is the 13-atom centered icosahedral unit. An icosahedron has 12 vertices, 20 triangular faces, and 30 edges. A hole is created that is capable of housing an additional "interior atom" of roughly 10% smaller in size than the "surface atoms". Thus, the metal–metal distances involving the three centroids of the three icosahedra (Au13, Au15, and Au17) are among the shortest (~2.74 Å) in the cluster **1**.

The idealized icosahedron belongs to the I_h point group, which has an inversion symmetry. Therefore, it should have six linear arrays of metal atoms. Indeed, each of the center atoms, Au13, Au15, and Au17, has six M–M–M bond angles (M = Au or Ag) close to linearity (>170°) (cf. Table III).

The spread of the distances around the icosahedral central atoms (for example, the distances of central Au13 to peripheral Au or Ag atoms range from 2.69 (1) Å for the Au13–Au7 bond to 2.87 (1) Å for the Au13–Au14 bond) indicates slight distortions of icosahedral unit away from the idealized icosahedral geometry and in large measure can be attributed to the distribution of different kinds of gold and silver atoms, and bonding and/or steric effects imposed by the $(Tol)_3P$ and the chlorine ligands.

If we focus our attention on the surface of an icosahedron, each of the 12 vertices is common to 5 triangular faces and 5 pentagonal cross sections. Thus the M–M–M angles on the surface of an ideal icosahedron must either be 60° or 108°. Indeed, Table III shows that all peripheral M–M–M (M = Au or Ag) angles in cluster **1** lie in the range of either 55.5–67.8° or 103.7–123.7° within each icosahedral unit.

D. 13-Atom Bicapped Pentagonal Prisms. The three shared vertices, Au14, Au16, and Au18, can be considered as centroids of three 13-atom bicapped pentagonal prisms.

A bicapped pentagonal prism belongs to D_{5h} symmetry with 12 vertices, 15 faces (10 triangles and 5 squares), and 25 edges. Since it does not have an inversion symmetry, there is only one linear array of three metal atoms. This is exactly what is observed: for example, only the bond angle of Au13–Au14–Au15 of 178.6 (4)° is close to linearity; all other angles centered around Au14 are 158° or smaller.

Unlike icosahedra, which have only triangular faces, bicapped pentagonal prisms have five square faces. This is indeed observed. For example, the four internal angles of the Ag1–Ag2–Ag4–Ag3 square are 99.4 (5)°, 81.1 (4)°, 97.4 (5)°, and 80.2 (4)°, with an average of 90°. Even the "squares" involving the shared vertices are not far from right angles; for example, the angles for Ag14–Ag16–Au16–Au18 (with the latter two atoms as shared vertices) are 89.1 (4)°, 95.5 (4)°, 90.0 (4)°, and 84.9 (4)°, again, with an average of 90°.

E. Nearly Close Packed Layers. Referring to Figure 2b, the 18 Au atoms are distributed approximately in three layers: 12 in the central layer denoted as the 0th layer and three each in layers ±1. The six central (type B) Ag atoms also lie in layers ±1. The 12 peripheral (type A) Ag atoms lie approximately halfway between layer 0 and layers ±1, which we shall call layers $\pm^1/_2$. Finally, the two exo-cluster apical (type C) Ag atoms are located in layers $\pm 2^1/_2$. Note that the two apical (type C) Ag atoms are located in layers $\pm 2^1/_2$ rather than ±2 because they are more distant from the cluster mainframe (cf. section III.B).

F. Terminal, Doubly, and Triply Bridging Halides. The 14 chloride ligands coordinate exclusively to the 20 Ag atoms. They are of three distinct types: six doubly bridging μ_2-Cl (connecting type A Ag atoms of adjacent icosahedra); six triply bridging μ_3-Cl (connecting type B and type C Ag atoms); and two terminal Cl (coordinated to type C Ag atoms). The coexistance of all three modes of bridging for the halide ligands in one cluster is rather interesting.

All Ag–Cl distances are normal. The averages (range in parentheses) of terminal, doubly, and triply bridging Ag–Cl distances are 2.37 (2.37–2.38), 2.44 (2.35–2.53), and 2.62 (2.51–2.73) Å, respectively.

One interesting observation is that the triply bridging chloride ligands have short Cl···Ag contacts of ca. 3.1 Å (e.g., Cl8···Ag8), which is significantly less than the sum (3.55 Å) of van der Waals radius of Cl (1.80 Å) and the atomic radius of Ag (1.75 Å). Though these distances are too long to be considered as normal covalent bonds, the tendency toward a quadruply bridging (μ_4) mode is noteworthy. It should be cautioned that this may be a manifestation of the tendency toward a more-or-less close packing of the chloride ligands over the silver layers.

The disposition of the 14 chloride ligands can be described as two nonbonding tetrahedra linked by three bridges. Alternatively, it can be described as a twisted trigonal prism (triply bridging halides Cl3, Cl4, Cl7, Cl8, Cl11, Cl12) with two triangular face caps (terminal halides Cl13 and Cl14). Concentric with this trigonal prism is another twisted trigonal prism (doubly bridging ligands Cl1,Cl2, Cl5, Cl6, Cl9, Cl10), which is shorter in height but larger in base area. Selected Cl···Cl contacts are tabulated in Table IV.

As shown in Figure 2b, the six doubly bridging chlorides are situated approximately in layers ±1 whereas the six triply bridging chlorides lie roughly in layers ±2. The terminal chlorides lie roughly in layers $\pm 3^1/_2$.

G. The Twelve Phosphines. Globally, the 12 tri(*p*-tolyl)-phosphine ligands, which coordinate to 12 peripheral Au atoms in a radial fashion (viz., away from the centered Au atoms of the three icosahedra), form a highly distorted twinned cuboctahedron. The nonbonding P···P distances are provided in Table V. Here, however, the central triangles of the distorted twinned cuboctahedron are enlarged since the phosphines are attached to the peripheral gold atoms only.

It is observed that the P atoms of six of the phosphine ligands

Table IV. Selected Nonbonding Cl···Cl Distances in the Cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$[a]

atom 1	atom 2	distance	atom 1	atom 2	distance
Cl1	Cl2	4.16 (5)	Cl6	Cl8	3.71 (5)
Cl1	Cl3	3.76 (5)	Cl7	Cl11	3.61 (5)
Cl2	Cl4	3.88 (4)	Cl7	Cl13	4.43 (5)
Cl3	Cl7	3.66 (4)	Cl8	Cl12	3.56 (5)
Cl3	Cl11	3.60 (5)	Cl8	Cl14	4.43 (5)
Cl3	Cl13	4.42 (5)	Cl9	Cl10	4.31 (5)
Cl4	Cl8	3.70 (3)	Cl9	Cl11	3.84 (6)
Cl4	Cl12	3.65 (5)	Cl10	Cl12	3.81 (5)
Cl4	Cl14	4.47 (5)	Cl11	Cl13	4.43 (5)
Cl5	Cl6	4.26 (5)	Cl12	Cl14	4.41 (5)
Cl5	Cl7	3.87 (4)			

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

Table V. Selected Nonbonding P···P Distances in the Cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$[a]

atom 1	atom 2	distance	atom 1	atom 2	distance
P1	P2	6.43 (6)	P4	P9	5.46 (4)
P1	P6	8.88 (4)	P4	P10	5.64 (5)
P1	P7	5.72 (6)	P5	P6	6.57 (5)
P1	P8	5.58 (6)	P5	P11	5.60 (5)
P2	P3	9.75 (6)	P5	P12	5.36 (5)
P2	P7	5.34 (5)	P6	P11	5.56 (6)
P2	P8	5.61 (5)	P6	P12	5.77 (5)
P3	P4	6.41 (4)	P7	P8	8.63 (5)
P3	P9	5.76 (5)	P9	P10	8.62 (5)
P3	P10	5.44 (5)	P11	P12	8.61 (5)
P4	P5	9.64 (5)			

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

(hereafter referred to as "equatorial" ligands) are roughly coplanar with the center layer of 12 Au atoms. Deviations of the P atoms from the least-squares planes of the Au atoms are tabulated in Table F (supplementary material). The remaining six P atoms (hereafter referred to as "axial" ligands), three above and three below the Au plane, lie approximately in layers ±2. The six equatorial P atoms are twisted slightly (viz., not exactly coplanar) giving rise to a "chair" conformation; these atoms, however, are roughly equidistant from the plane of the 12 central Au atoms [cf. Table F (supplementary material)].

If we focus our attention on the individual icosahedron, we see that the four peripheral Au atoms, for example, Au1, Au2, Au7, Au8, along with the central atom Au13, form a trigonal bipyramid. The four phosphine ligands are coordinated to the four peripheral Au atoms as follows: P1 and P2 (coordinated to Au1 and Au2) occupy the equatorial positions while P7 and P8 (coordinated to Au7 and Au8) occupy the axial positions.

The 12 phosphine ligands can be divided into two classes in terms of bond lengths and angles. The difference of bond lengths between the two kinds of phosphine ligands is reflected in (cf. Table II) the shorter Au–P(axial) bond lengths (in the range of 2.29–2.34 Å, with an average of 2.31 Å) compared to the Au–P(equatorial) bond lengths (2.35–2.47 Å, with an average of 2.40 Å). All the Au(central)–Au(peripheral)–P moieties are essentially linear, although the degree of their slight bending is significant enough to tell the difference between equatorial and axial phosphines. The Au(central)–Au(peripheral)–P(equatorial) angles span the range of 161.7–171.0°. These values deviate significantly from linearity. The corresponding Au(central)–Au(peripheral)–P(axial) angles deviate less from linearity, which lies in the range of 177–179.3°. We believe that the larger deviation of the Au–Au–P angles from linearity and the longer Au–P bond lengths for the equatorial phosphines are manifestations of steric repulsions between adjacent phosphine ligands in the equatorial plane.

The 36 Au–P–C angles, ranging from 110° to 125° (with a few exceptions), are greater than the ideal tetrahedral angle whereas the 36 C–P–C angles, ranging from 100° to 115°, are signficantly smaller (cf. Table VII). An interesting pattern is also observed for the P–C–C (cf. Table VII): viz., those oriented

Table VI. P–C(tolyl) Distances in the Cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$[a]

atom 1	atom 2	distance	atom 1	atom 2	distance
P1	C1C1	1.62 (4)	P7	C7A1	1.60 (3)
P1	C1A1	1.83 (5)	P7	C7B1	1.76 (4)
P1	C1B1	1.81 (5)	P7	C7C1	1.97 (4)
P2	C2A1	1.82 (5)	P8	C8A1	1.87 (4)
P2	C2B1	1.78 (5)	P8	C8C1	1.67 (5)
P2	C2C1	1.84 (5)	P8	C8B1	1.82 (4)
P3	C3C1	1.54 (5)	P9	C9A1	1.68 (5)
P3	C3A1	1.66 (4)	P9	C9C1	1.95 (3)
P3	C3B1	1.67 (4)	P9	C9B1	1.78 (4)
P4	C4A1	1.72 (4)	P10	C10A1	1.74 (5)
P4	C4B1	1.57 (5)	P10	C10B1	1.90 (3)
P4	C4C1	1.85 (4)	P10	C10C1	1.79 (4)
P5	C5C1	1.65 (4)	P11	C11B1	1.90 (4)
P5	C5A1	1.85 (4)	P11	C11A1	1.69 (5)
P5	C5B1	1.71 (4)	P11	C11C1	1.83 (4)
P6	C6C1	1.88 (4)	P12	C12A1	1.88 (4)
P6	C6B1	1.65 (4)	P12	C12B1	1.79 (4)
P6	C6A1	1.86 (4)	P12	C12C1	1.46 (4)

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

toward the pseudo-3-fold axis of the $(Tol)_3P$ are all greater than the ideal trigonal angle of 120° whereas those oriented in the opposite direction are somewhat smaller. These observations for cluster **1** are very similar to those observed in the cubane-like $(Ph_3P)_4M_4X_4$ (M = Cu, Ag; and X = Cl, Br, I).[15]

H. Highly Disordered Solvent Molecules. Since large metal clusters of interest here are beginning to approach the size of small proteins, it is not surprising that X-ray structural determination of these large "small" molecules carries the same problems often encountered in the small "large" molecules of proteins. The solvent molecules are highly disordered and/or lost during data collection as a result of crystal decay. Consequently, only 125 atoms with electron densities greater than 1.0 e/Å^3 were found in the difference Fourier map. In some cases, solvents are associated by hydrogen bonding or weak O–H···Cl (or C–H···Cl) or weak O–H···C_{ring} (or C–H···C_{ring}) interactions with cluster **1**. Interatomic distances corresponding to shorter than normal van der Waals contacts of cluster **1** and solvents (O–H···Cl or C–H···Cl ≥ 2.8 and ≤ 3.8 Å, and O–H···C_{ring} or C–H···C_{ring} ≥ 2.6 and ≤3.4 Å) are summarized in Table G (supplementary material). The formula, therefore, is approximately **1**·42EtOH. However, not all of these solvent molecules are of unit weight. Some are lost during data collection; some are smeared out due to disorder and/or liquidlike arrangement. As described previously, such disorder was modeled by first refining the occupancy of the solvent atoms with a fixed isotropic temperature factor of 8 Å^2 (roughly the average of the tolyl groups), followed by refining the isotropic thermal parameter while holding the occupancy fixed. By adding up the occupancies (weight), a total of 37 EtOH molecules per asymmetric unit can be obtained. The final formula for the crystal with which the data were collected, therefore, is approximately **1**·37EtOH. Owing to the highly disordered nature of the solvent molecules, no attempts were made to interpret their bond lengths and angles.

I. Empirical Structural Rules for the Au–Ag Supraclusters. A close examination of the structure of cluster **1** and related clusters revealed that there are certain empirical rules in the formation of these clusters: (1) the halide ligands are bonded to the silver atoms; (2) the phosphine ligands are attached to the gold atoms; (3) the "interstitial" or "bulk" atom in the icosahedral cages are gold atoms; and (4) the "shared" vertices (bicapped pentagonal prismatic cages) are also gold atoms.

These rules may explain why the structures of this class of Au–Ag clusters are ordered (rather than a statistical distribution of Au and Ag atoms within the metal framework) despite the fact that Au and Ag are roughly equal in size and completely miscible in the alloy solid solution.

(15) Teo, B. K.; Calabrese, J. C. *Inorg. Chem.* **1976**, *15*, 2467.

Table VII. Au–P–C, C–P–C, and P–C–C Angles in the Cluster $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$[a]

atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle	atom 1	atom 2	atom 3	angle
Au1	P1	C1C1	125 (3)	Au4	P4	C4A1	110 (2)	Au7	P7	C7A1	117 (2)	Au10	P10	C10A1	115 (2)
Au1	P1	C1A1	104 (2)	Au4	P4	C4B1	117 (2)	Au7	P7	C7B1	111 (2)	Au10	P10	C10B1	110 (2)
Au1	P1	C1B1	110 (2)	Au4	P4	C4C1	103 (2)	Au7	P7	C7C1	115 (1)	Au10	P10	C10C1	110 (2)
C1C1	P1	C1A1	103 (3)	C4A1	P4	C4B1	100 (2)	C7A1	P7	C7B1	102 (2)	C10A1	P10	C10B1	100 (2)
C1C1	P1	C1B1	105 (3)	C4A1	P4	C4C1	115 (2)	C7A1	P7	C7C1	102 (2)	C10A1	P10	C10C1	104 (2)
C1A1	P1	C1B1	108 (2)	C4B1	P4	C4C1	113 (2)	C7B1	P7	C7C1	108 (2)	C10B1	P10	C10C1	117 (2)
Au2	P2	C2A1	110 (2)	Au5	P5	C5C1	99 (2)	Au8	P8	C8A1	115 (2)	Au11	P11	C11B1	112 (2)
Au2	P2	C2B1	117 (2)	Au5	P5	C5A1	116 (2)	Au8	P8	C8C1	110 (3)	Au11	P11	C11A1	109 (2)
Au2	P2	C2C1	112 (2)	Au5	P5	C5B1	116 (2)	Au8	P8	C8B1	112 (2)	Au11	P11	C11C1	116 (2)
C2A1	P2	C2B1	105 (2)	C5C1	P5	C5A1	111 (2)	C8A1	P8	C8C1	107 (2)	C11B1	P11	C11A1	110 (2)
C2A1	P2	C2C1	109 (3)	C5C1	P5	C5B1	109 (2)	C8A1	P8	C8B1	105 (3)	C11B1	P11	C11C1	102 (2)
C2B1	P2	C2C1	103 (2)	C5A1	P5	C5B1	106 (2)	C8C1	P8	C8B1	109 (2)	C11A1	P11	C11C1	107 (2)
Au3	P3	C3C1	113 (2)	Au6	P6	C6C1	123 (2)	Au9	P9	C9A1	116 (2)	Au12	P12	C12A1	115 (2)
Au3	P3	C3A1	108 (2)	Au6	P6	C6B1	113 (2)	Au9	P9	C9C1	115 (2)	Au12	P12	C12B1	112 (2)
Au3	P3	C3B1	109 (2)	Au6	P6	C6A1	101 (2)	Au9	P9	C9B1	111 (2)	Au12	P12	C12C1	112 (2)
C3C1	P3	C3A1	107 (3)	C6C1	P6	C6B1	104 (2)	C9A1	P9	C9C1	104 (2)	C12A1	P12	C12B1	101 (2)
C3C1	P3	C3B1	113 (3)	C6C1	P6	C6A1	103 (2)	C9A1	P9	C9B1	106 (2)	C12A1	P12	C12C1	100 (2)
C3A1	P3	C3B1	108 (2)	C6B1	P6	C6A1	112 (2)	C9C1	P9	C9B1	104 (2)	C12B1	P12	C12C1	116 (2)
P1	C1C1	C1C2	113 (2)	P4	C4C1	C4C2	106 (1)	P7	C7C1	C7C2	112 (1)	P10	C10B1	C10B2	129 (2)
P1	C1A1	C1A6	117 (2)	P4	C4C1	C4C6	134 (1)	P7	C7C1	C7C6	127.7 (9)	P10	C10B1	C10B6	108 (2)
P1	C1B1	C1B2	118 (2)	P5	C5A1	C5A2	126 (1)	P8	C8C1	C8C2	113 (2)	P11	C11C1	C11C2	127 (1)
P2	C2B1	C2B6	117 (1)	P5	C5A1	C5A6	113 (1)	P8	C8C1	C8C6	127 (2)	P11	C11C1	C11C6	113 (1)
P2	C2A1	C2A2	124 (1)	P5	C5B1	C5B2	117 (1)	P8	C8A1	C8A2	123 (2)	P11	C11A1	C11A2	108 (1)
P2	C2A1	C2A6	116 (1)	P5	C5B1	C5B6	123 (1)	P8	C8A1	C8A6	117 (2)	P11	C11A1	C11A6	132 (1)
P2	C2C1	C2C2	130 (2)	P5	C5C1	C5C2	115 (1)	P8	C8B1	C8B2	122 (1)	P9	C9C1	C9C6	124 (1)
P2	C2C1	C2C6	110 (2)	P5	C5C1	C5C6	124 (1)	P8	C8B1	C8B6	118 (1)	P9	C9A1	C9A2	116 (1)
P3	C3C1	C3C2	120 (1)	P6	C6B1	C6B2	109 (2)	P9	C9C1	C9C2	116 (1)	P9	C9A1	C9A6	124 (1)
P3	C3C1	C3C6	118 (1)	P6	C6B1	C6B6	130 (2)	P6	C6C1	C6C2	123 (1)	P9	C9B1	C9B2	122 (1)
P3	C3A1	C3A2	125 (1)	P6	C6A1	C6A2	118 (1)	P6	C6C1	C6C6	117 (1)	P12	C12C1	C12C2	116 (2)
P3	C3A1	C3A6	115 (1)	P6	C6A1	C6A6	122 (1)	P7	C7B1	C7B2	123 (1)	P12	C12C1	C12C6	124 (2)
P3	C3B1	C3B2	116 (2)	P4	C4A1	C4A2	122 (2)	P7	C7B1	C7B6	117 (1)	P11	C11B1	C11B2	120 (1)
P3	C3B1	C3B6	124 (2)	P4	C4A1	C4A6	118 (2)	P9	C9B1	C9B6	117 (1)	P11	C11B1	C11B6	118 (1)
P1	C1C1	C1C6	127 (2)	P4	C4B1	C4B2	112 (1)	P10	C10A1	C10A2	122 (1)	P12	C12A1	C12A2	118 (1)
P1	C1A1	C1A2	123 (2)	P4	C4B1	C4B6	127 (1)	P10	C10A1	C10A6	117 (1)	P12	C12A1	C12A6	122 (1)
P1	C1B1	C1B6	122 (2)	P7	C7A1	C7A2	114 (1)	P10	C10C1	C10C2	121 (1)	P12	C12B1	C12B2	127 (1)
P2	C2B1	C2B2	123 (1)	P7	C7A1	C7A6	125 (1)	P10	C10C1	C10C6	119 (1)	P12	C12B1	C12B6	113 (1)

[a] Numbers in parentheses are estimated standard deviations in the least significant digits.

J. Crystal Structure. The crystal structure of the title compound is composed of two cluster **1** and 84 highly disordered, liquidlike EtOH molecules per unit cell. Since the space group is $P\bar{1}$, the crystallographically independent asymmetric unit comprises **1**·42EtOH.

The centroid of cluster **1** resides at (0.486, 0.179, 0.306) with the idealized 3-fold axis (the Ag19–Ag20 vector) lying approximately parallel to the crystallographic a axis. As a result, the central layer (layer 0) of the cluster lies close to $x = 0.48$ plane. Furthermore, the Au13–Au14–Au15 edge of the central ν_2 gold triangle is nearly parallel to the crystallographic b axis. Finally, it is interesting to point out that the coordinates of Ag19 and Ag20 differ only in $\Delta x \approx 0.5$.

K. Electron Counting. We recently proposed a cluster of clusters (C^2) model for the electron counting of superclusters based on vertex-, edge-, or face-sharing of smaller cluster units as building blocks.[4]

The title cluster **1** can be considered as a 36-atom cluster, formed by three 13-atom icosahedra sharing three vertices in a cyclic manner, plus two exopolyhedral Ag atoms. By use of the C^2 approach, the number of skeletal electron pairs for the 36-atom cluster mainframe is $B = (3 \times 13)$ (three icosahedra) $- (3 \times 3)$ (sharing three vertices) $= 30$. Since the number of "surface atoms" is $V_m = 36 - 3$ (three centroids) $= 33$, the total number of electron pairs is $T = 6V_m + B = 6 \times 33 + 30 = 228$. Since the two exopolyhedral Ag atoms (Ag19 and Ag20) do not form metal–metal bonds with the 36-atom polyhedral framework (Ag···Ag distances ranging from 3.69 to 3.80 Å with an average of 3.73 Å), one can consider that each of these two Ag atoms contributes nine electron pairs (viz., 18 electrons satisfying the effective atom number rule) to the cluster bonding. Thus the total number of electron pairs for the 38-atom cluster **1** will be $T = 228 + (2 \times 9) = 246$. The predicted electron count is $N = 2T = 2 \times 246 = 492$. This is in good agreement with the observed electron count of $N_{obs} = (12 \times 2)$ (phosphine) $+ (38 \times 11)$ (metal) $+ (2 \times 1)$ (terminal Cl) $+ (6 \times 3)$ (doubly bridging Cl) $+ (6 \times 5)$ (triply bridging Cl) $= 492$.

It is tempting to predict that if one or both of the exopolyhedral Ag atoms begin to form three or six metal–metal bonds with the polyhedral cluster framework, the electron counts will become $N = 492 - (3 \times 2) = 486$ and $N = 492 - (6 \times 2) = 480$, respectively.

Acknowledgment is made to the National Science Foundation (CHE-8722339), and the donors of the Petroleum Research Fund, administered by the American Chemical Society, for financial support of this research. We are also grateful to the University of Illinois at Chicago for a Campus Research Board Award. We would also like to express our sincere gratitude to Professor C. Strouse of UCLA for generously providing the rigid-body program and making helpful suggestions for the modification of the crystallographic programs, and to Drs A. Syed, K. Fay, and G. Williams of Enraf-Nonius for their generous help in the modification of the SDP programs.

Registry No. 1, 114654-93-2; **1**·42EtOH, 129647-93-4; $(p\text{-Tol})_3PAuCl$, 28978-10-1; $[(p\text{-Tol})_3PAgCl]_4$, 129467-07-8.

Supplementary Material Available: Full listings for $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$ of positional parameters and equivalent isotropic thermal parameters (Table A), anisotropic thermal parameters (Table B), positional and orientational parameters of the tolyl groups (Table C), positional and isotropic thermal parameters of individual carbon atoms in the tolyl groups (Table D), atomic positional parameters and equivalent isotropic displacement parameters of solvent atoms (Table E), least-squares planes and distances from the planes of selected groups of atoms (Table F), and selected intra- and intermolecular van der Waals contacts (Table G) (27 pages); listing of observed and calculated structure factors (Table H) for $(p\text{-Tol}_3P)_{12}Au_{18}Ag_{20}Cl_{14}$·42EtOH (47 pages). Ordering information is given on any current masthead page.