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

Tuning the electronic structure of gold cluster-assembled materials by altering organophosphine ligands

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SUPPORTING INFORMATION

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1. DFT geometry relaxation of $Au_{32}(^nBu_3P)_{12}Cl_8$ system

Table S 1. Lattice parameters (a, b, c, in Å; α, β, γ, in degrees) and unit-cell volume (in Å^3) for ***$Au_{32}(^nBu_3P)_{12}Cl_8$*** *system as obtained by a full structure relaxation with the PBE-D3, PBEsol, and PBE functionals. The lattice parameters are compared to the corresponding experimental values (Exp.). The relative deviations (Dev, in %) are estimated as $Value^{exp}$ – $Value^{theor}$ divided by $Value^{exp}$ (where $Value^{theor}$ stands for the lattice parameter obtained at the PBE-D3 or PBEsol levels of theory).*

	PBE-D3	**PBEsol**	**PBE**	**Exp.** [1, 2]
a (Å)	32.86	33.20	34.02	33.29
Dev(a) (in %)	-1.30	-0.28	2.19	-
b (Å)	18.98	19.08	19.43	19.08
Dev(b) (in %)	-0.53	-0.03	1.80	-
c (Å)	19.31	19.40	19.78	19.34
Dev(c) (in %)	-0.14	0.34	2.29	-
α (°)	63.38	63.34	63.28	63.44
Dev(α) (in %)	-0.08	-0.15	-0.24	-
β (°)	77.73	72.64	72.59	72.98
Dev(β) (in %)	6.51	-0.47	-0.54	-
γ (°)	77.73	77.75	77.80	78.30
Dev(γ) (in %)	-0.72	-0.70	-0.63	-
Unit cell volume (Å^3)	10237	10437	11097	10470
Dev(Unit cell volume) (in %)	-2.22	-0.31	5.99	-

2. The density of states (DOS) of lattice structures and singlet state clusters

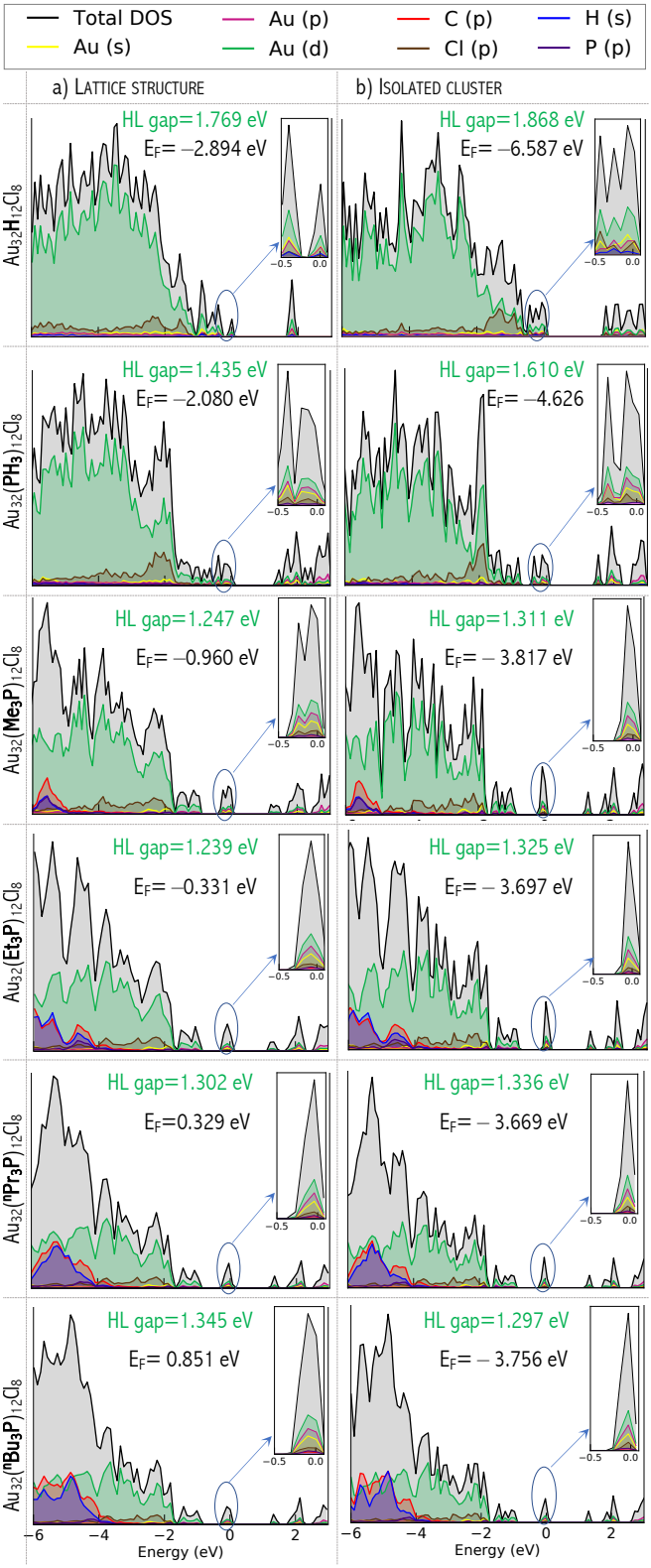

Figure S 1 *The total density of states (TDOS) and partial density of states (PDOS) for (a) the lattice structure and (b) isolated $Au_{32}\boldsymbol{H}_{12}Cl_8$ and $Au_{32}\boldsymbol{(R_3P)}_{12}Cl_8$ singlet spin state clusters as obtained from PBE0-D3 and energy cutoff of 520 eV. Zero energy (E=0) is set to the valence band maximum (VBM).*

3. Molecular orbitals of isolated clusters

The equilibrium geometries of isolated clusters were obtained at the PBEsol theory level using the Vienna *ab initio* simulation package (VASP, Rev.6.3.2). [3-6] Subsequently, molecular orbitals were obtained using Gaussian 16 software [7] and PBE0-D3 method with the 6-31++G(d,p) basis sets at the equilibrium geometries optimized at the PBEsol level (incorporated in VASP Rev.6.3.2 software). [3-6] For the gold atoms, the Los Alamos National Laboratory (LANL) effective core potentials (ECP) with the appropriate valence basis set of double-ζ quality (denoted LANL2DZ) [8, 9] was employed.

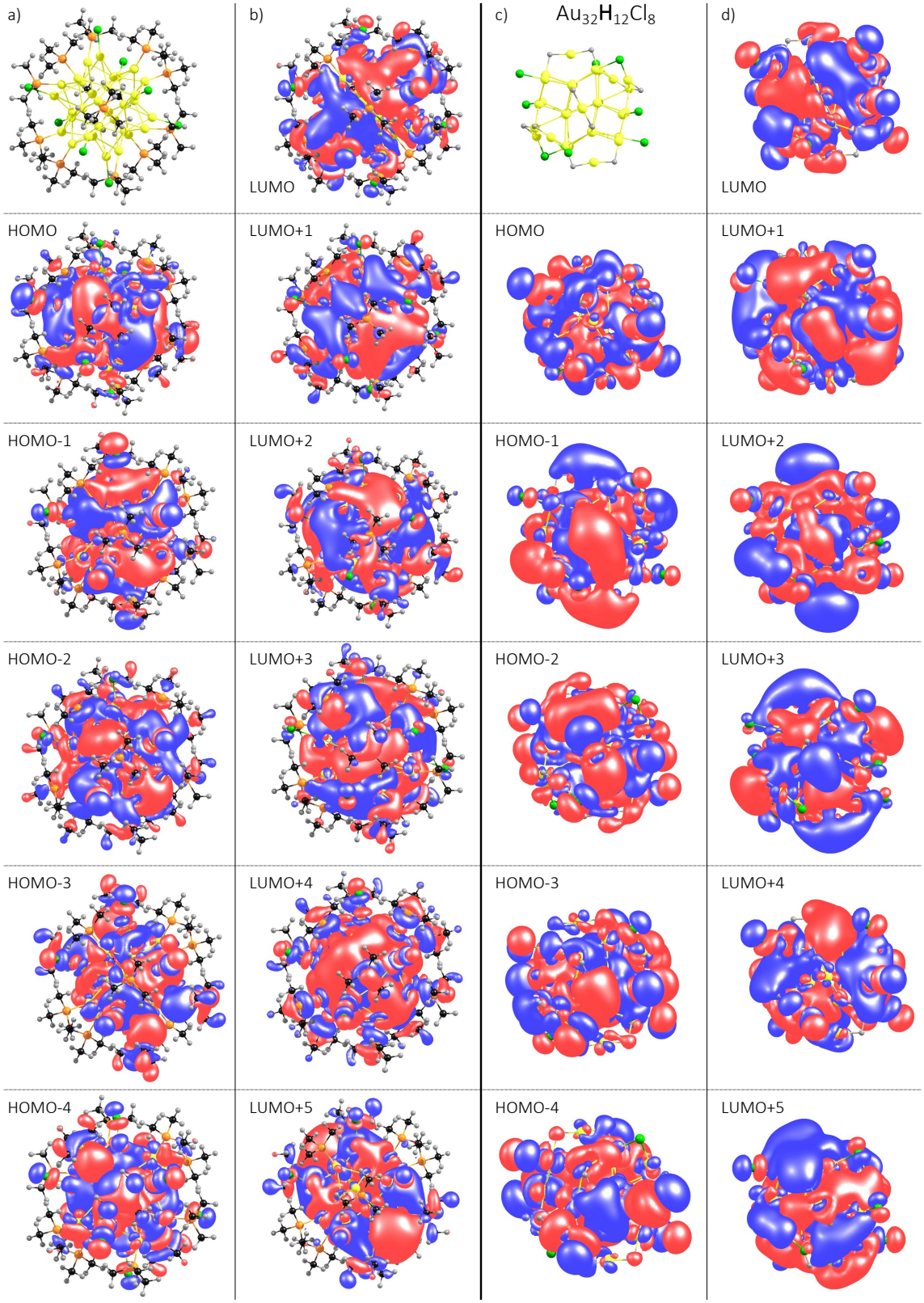

Figure S 2 The highest occupied molecular orbitals (HOMOs) and the lowest unoccupied molecular orbitals (LUMOs) of the singlet spin state (a-b) $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ and (c-d) $Au_{32}\mathbf{H}_{12}Cl_8$ isolated cluster as obtained from the PBE0-D3/6-31++G(d,p)+LanL2DZ using Gaussian 16 software.

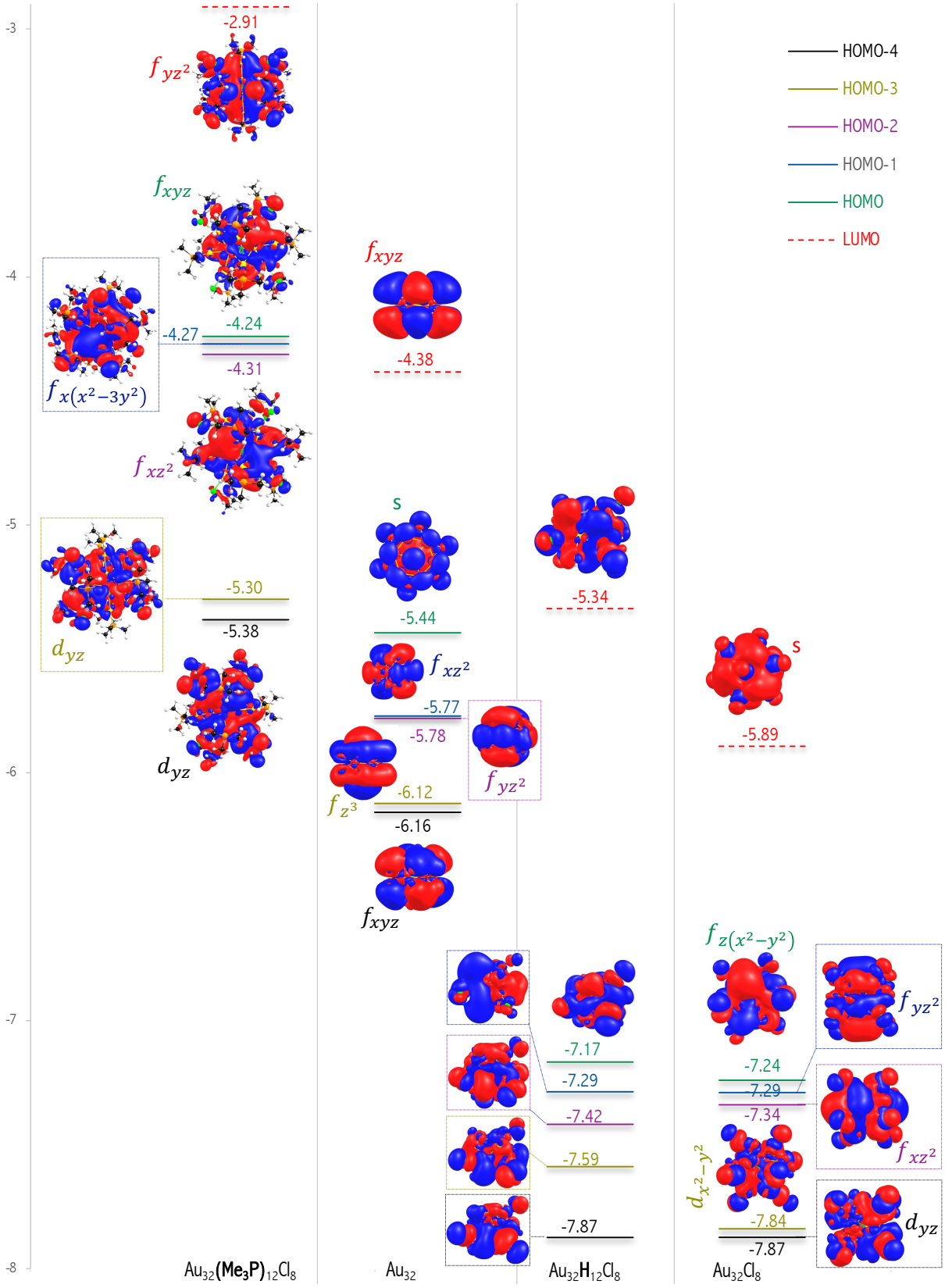

Figure S 3 The PBE0-D3/6-31++G(d,p)+LanL2DZ energy diagrams of $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ (first column), Au_{32} (second column), $Au_{32}H_{12}$ (third column), and $Au_{32}Cl_8$ (fourth column). All equilibrium structures correspond to singlet spin states. The solid and red dashed lines represent the occupied and unoccupied energy levels, respectively.

4. Au-Au distances in Au_{32} fragment of bare and ligated clusters

We obtained the average Au-Au bond lengths (in Å) of the Au_{12} core, Au_{20} shell, and core-shell distances for $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$, Au_{32}, and $Au_{32}\mathbf{H}_{12}Cl_8$ isolated clusters. *Figure S 4* shows the average bond lengths of singlet spin state equilibria. The average bond lengths are overages of PBEsol/6-31++G(d,p)+LanL2DZ bond lengths (depicted in Table S 2). The structure of $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ and $Au_{32}\mathbf{H}_{12}Cl_8$ isolated clusters with representative bond lengths are depicted in Figure S 5.

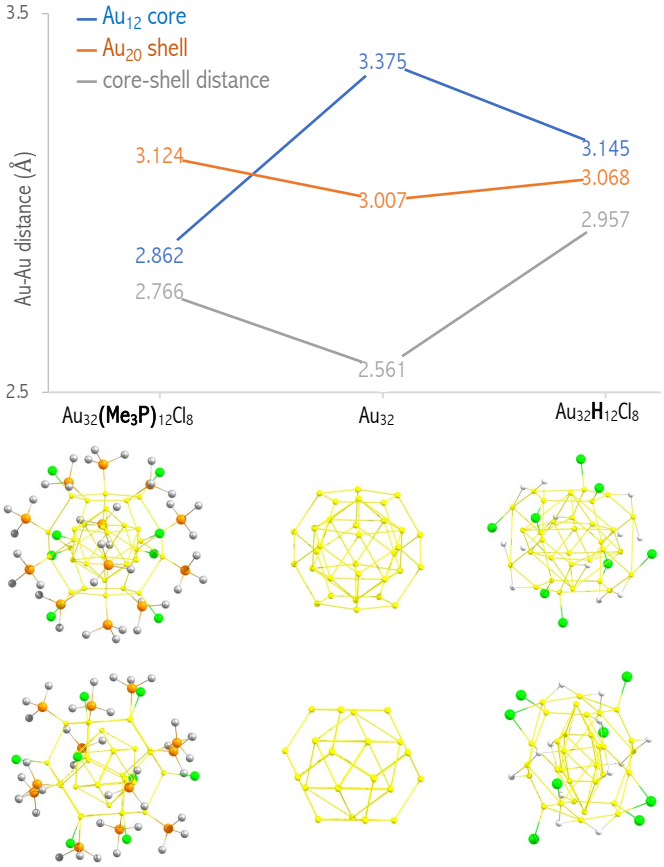

Figure S 4 The average Au-Au bond lengths (in Å) of Au_{12} core (blue line), Au_{20} shell (orange line), and core-shell distances (grey line) obtained for $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ (left column), Au_{32} (middle column), and $Au_{32}H_{12}$ singlet spin state (right column). In the $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ structure hydrogen atoms are omitted for clarity.

Table S 2. *The PBEsol/6-31++G(d,p)+LanL2DZ Au-Au bond lengths (in Å) of Au_{12} core (blue values), Au_{20} shell (orange values), and core-shell distances (green values) for $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$, Au_{32}, and $Au_{32}\mathbf{H_{12}}Cl_8$ isolated clusters.*

$Au_{32}(\mathbf{Me_3P})_{12}Cl_8$					Au_{32}					$Au_{32}\mathbf{H}_{12}Cl_8$ Singlet					$Au_{32}H_{12}Cl_8$ Triplet				
Name	Atom1	Atom2	Mult	Distance	Name	Atom 1	Atom 2	Mult	Distance	Name	Atom 1	Atom 2	Mult	Distance	Name	Atom 1	Atom 2	Mult	Distance
AuAu	10	12	2	2.822	AuAu	10	12	2	2.723	AuAu	18	22	2	2.659	AuAu	1	5	1	2.7125
AuAu	8	12	6	2.828	AuAu	9	11	1	2.724	AuAu	3	21	2	2.750	AuAu	17	21	1	2.7245
AuAu	1	3	2	2.831	AuAu	8	10	3	2.787	AuAu	5	6	2	2.764	AuAu	2	6	1	2.7342
AuAu	1	8	2	2.839	AuAu	2	12	2	2.792	AuAu	17	21	2	2.813	AuAu	18	22	1	2.7379
AuAu	6	9	2	2.844	AuAu	8	12	1	3.713	AuAu	20	22	2	2.848	AuAu	1	6	2	2.7617
AuAu	2	10	2	2.857	AuAu	6	12	1	3.716	AuAu	2	20	2	2.882	AuAu	6	21	4	2.7702
AuAu	3	5	2	2.861	AuAu	2	4	1	3.732	AuAu	20	21	2	2.883	AuAu	20	22	3	2.794
AuAu	3	8	2	2.875	AuAu	3	8	1	3.741	AuAu	17	18	2	2.901	AuAu	4	22	1	2.8413
AuAu	2	5	2	2.881	AuAu	1	3	1	3.755	AuAu	19	22	2	2.927	AuAu	6	20	1	2.8547
AuAu	5	11	2	2.900	AuAu	6	9	1	3.763	AuAu	19	20	2	3.264	AuAu	20	21	1	3.0499
AuAu	5	7	2	2.912	AuAu	5	11	1	3.767	AuAu	5	18	2	3.938	AuAu	4	5	1	3.0735
AuAu	2	12	2	2.965	AuAu	2	10	2	3.769	AuAu	3	17	2	4.174	AuAu	4	17	1	3.2198
AuAu	15	28	2	2.885	AuAu	5	10	1	3.794	AuAu	18	19	2	4.430	AuAu	3	21	1	3.2408
AuAu	19	21	2	2.904	AuAu	4	7	1	3.810	AuAu	31	32	4	2.648	AuAu	1	20	1	3.2579
AuAu	14	30	2	2.937	AuAu	7	11	1	3.830	AuAu	12	13	2	2.664	AuAu	5	19	2	3.2698
AuAu	24	26	2	2.974	AuAu	18	20	1	2.774	AuAu	27	28	2	2.680	AuAu	1	2	1	3.3037
AuAu	29	31	2	3.067	AuAu	13	15	4	2.776	AuAu	14	16	2	2.682	AuAu	2	21	1	3.8692
AuAu	18	20	2	3.118	AuAu	20	22	2	2.779	AuAu	8	9	2	2.718	AuAu	5	18	1	3.9074
AuAu	17	25	2	3.122	AuAu	29	31	1	2.780	AuAu	23	24	2	2.748	AuAu	3	6	1	3.939
AuAu	23	27	2	3.148	AuAu	30	32	4	2.782	AuAu	10	32	2	2.757	AuAu	4	20	1	3.962
AuAu	25	29	2	3.153	AuAu	14	16	1	2.791	AuAu	8	30	2	2.835	AuAu	19	22	1	4.01
AuAu	13	15	2	3.204	AuAu	15	17	3	2.794	AuAu	26	27	2	2.862	AuAu	6	22	1	4.0175
AuAu	20	31	2	3.237	AuAu	23	25	2	2.797	AuAu	11	23	2	3.537	AuAu	3	4	1	4.5576
AuAu	15	17	2	3.249	AuAu	16	18	1	2.799	AuAu	13	15	2	3.579	AuAu	7	15	2	2.6377
AuAu	27	31	1	3.264	AuAu	23	27	4	2.805	AuAu	7	15	2	3.676	AuAu	23	31	1	2.6452
AuAu	28	32	1	3.265	AuAu	18	26	1	2.813	AuAu	9	10	2	3.859	AuAu	15	16	1	2.6515
AuAu	21	23	2	3.288	AuAu	2	18	2	2.635	AuAu	28	30	2	4.124	AuAu	31	32	1	2.6535
AuAu	14	21	2	3.315	AuAu	5	14	3	2.637	AuAu	4	26	2	2.637	AuAu	12	13	1	2.6728
AuAu	1	13	2	2.687	AuAu	2	14	1	2.643	AuAu	18	25	4	2.693	AuAu	8	9	1	2.6748
AuAu	12	24	2	2.689	AuAu	8	17	2	2.646	AuAu	4	14	2	2.704	AuAu	30	32	1	2.6799
AuAu	11	31	2	2.696	AuAu	6	28	1	2.648	AuAu	21	23	4	2.722	AuAu	28	29	1	2.6864
AuAu	2	18	2	2.713	AuAu	7	27	1	2.649	AuAu	3	14	2	2.743	AuAu	24	25	1	2.6883
AuAu	6	15	2	2.722	AuAu	1	13	1	2.652	AuAu	3	12	2	2.755	AuAu	18	29	1	2.774
AuAu	5	27	4	2.724	AuAu	7	18	1	2.656	AuAu	3	11	2	2.766	AuAu	27	28	1	2.7839
AuAu	3	19	2	2.727	AuAu	4	26	1	2.700	AuAu	10	21	2	2.770	AuAu	16	26	1	2.8235
AuAu	9	29	2	2.743	AuAu	10	21	2	2.703	AuAu	22	28	2	2.799	AuAu	10	32	1	2.8286
AuAu	3	21	2	2.750	AuAu	10	30	1	2.707	AuAu	20	32	2	2.811	AuAu	10	11	2	2.8633

AuAu	8	28	4	2.758	AuAu	11	23	2	2.709	AuAu	22	32	2	2.836	AuAu	26	27	1	2.8674
AuAu	10	21	2	2.759	AuAu	3	25	1	2.714	AuAu	17	25	2	2.839	AuAu	14	24	1	2.9438
AuAu	10	19	4	2.761	AuAu	12	24	4	2.716	AuAu	18	26	2	2.852	AuAu	8	30	1	2.9463
AuAu	7	18	2	2.773	AuAu	4	20	3	2.720	AuAu	17	23	2	2.921	AuAu	23	24	1	2.9504
AuAu	2	30	2	2.777	AuAu	2	30	1	2.730	AuAu	5	16	2	2.938	AuAu	7	8	1	2.9528
AuAu	10	32	1	2.779	AuAu	5	23	2	2.733	AuAu	2	12	2	2.954	AuAu	10	31	1	3.1619
AuAu	10	14	5	2.779	AuAu	7	16	1	2.735	AuAu	4	25	2	3.013	AuAu	7	27	3	3.1651
AuAu	8	32	2	2.784	AuAu	2	26	1	2.738	AuAu	11	21	2	3.221	AuAu	15	26	1	3.2053
AuAu	4	24	2	2.785	AuAu	8	15	2	2.741	AuAu	22	29	2	3.278	AuAu	11	23	1	3.2247
AuAu	11	29	4	2.792	AuAu	7	20	4	2.744	AuAu	21	31	2	3.305	AuAu	28	30	1	3.474
AuAu	1	25	2	2.799	AuAu	10	32	2	2.746	AuAu	22	30	2	3.360	AuAu	12	14	1	3.524
AuAu	7	20	4	2.808	AuAu	6	15	1	2.747	AuAu	22	31	2	3.394	AuAu	15	27	1	3.9771
AuAu	6	22	2	2.810	AuAu	5	16	2	2.748	AuAu	2	11	2	3.409	AuAu	19	27	1	2.6295
AuAu	6	13	2	2.815	AuAu	7	31	2	2.752	AuAu	1	13	2	3.515	AuAu	2	9	1	2.661
AuAu	12	28	4	2.849	AuAu	5	21	2	2.753	AuAu	5	8	2	3.622	AuAu	18	25	1	2.6624
					AuAu	11	29	2	2.756	AuAu	4	24	2	2.782	AuAu	4	26	1	2.6641
					AuAu	10	19	1	2.758	AuAu	1	8	2	2.815	AuAu	10	20	2	2.6687
					AuAu	6	22	1	2.760	AuAu	2	13	2	2.829	AuAu	3	12	1	2.6841
					AuAu	11	25	1	2.766						AuAu	19	28	1	2.7017
					AuAu	3	23	2	2.769						AuAu	20	30	2	2.7317
					AuAu	12	30	2	2.771						AuAu	6	16	1	2.7487
					AuAu	9	20	1	2.773						AuAu	22	32	1	2.753
					AuAu	12	28	1	2.784						AuAu	20	32	4	2.7566
					AuAu	8	10	3	2.787						AuAu	4	16	1	2.7635
					AuAu	9	13	4	2.790						AuAu	22	28	1	2.7648
					AuAu	3	17	1	2.798						AuAu	21	24	1	2.7676
															AuAu	22	30	2	2.7896
															AuAu	1	8	2	2.7982
															AuAu	17	24	1	2.8023
															AuAu	6	14	1	2.8038
															AuAu	18	26	1	2.8133
															AuAu	2	12	1	2.8176
															AuAu	18	28	1	2.8345
															AuAu	2	10	2	2.8442
															AuAu	4	24	2	2.8464
															AuAu	4	25	1	2.8593
															AuAu	8	20	1	2.8714
															AuAu	3	14	1	2.9184
															AuAu	19	30	1	2.9221
															AuAu	21	23	1	2.9247
															AuAu	1	15	1	2.927
															AuAu	5	7	1	2.9326

AuAu	17	31	1	2.945		
AuAu	11	21	1	2.9781		
AuAu	5	27	1	2.9953		
AuAu	22	29	1	3.0098		
AuAu	21	31	1	3.0149		
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AuAu	17	25	1	3.1121		
AuAu	1	9	1	3.1307		
AuAu	17	23	1	3.2304		
AuAu	1	7	1	3.2343		
AuAu	1	13	1	3.2767		
AuAu	17	29	1	3.2925		
AuAu	5	16	1	3.3804		
AuAu	21	32	1	3.4038		
AuAu	7	19	1	3.4084		
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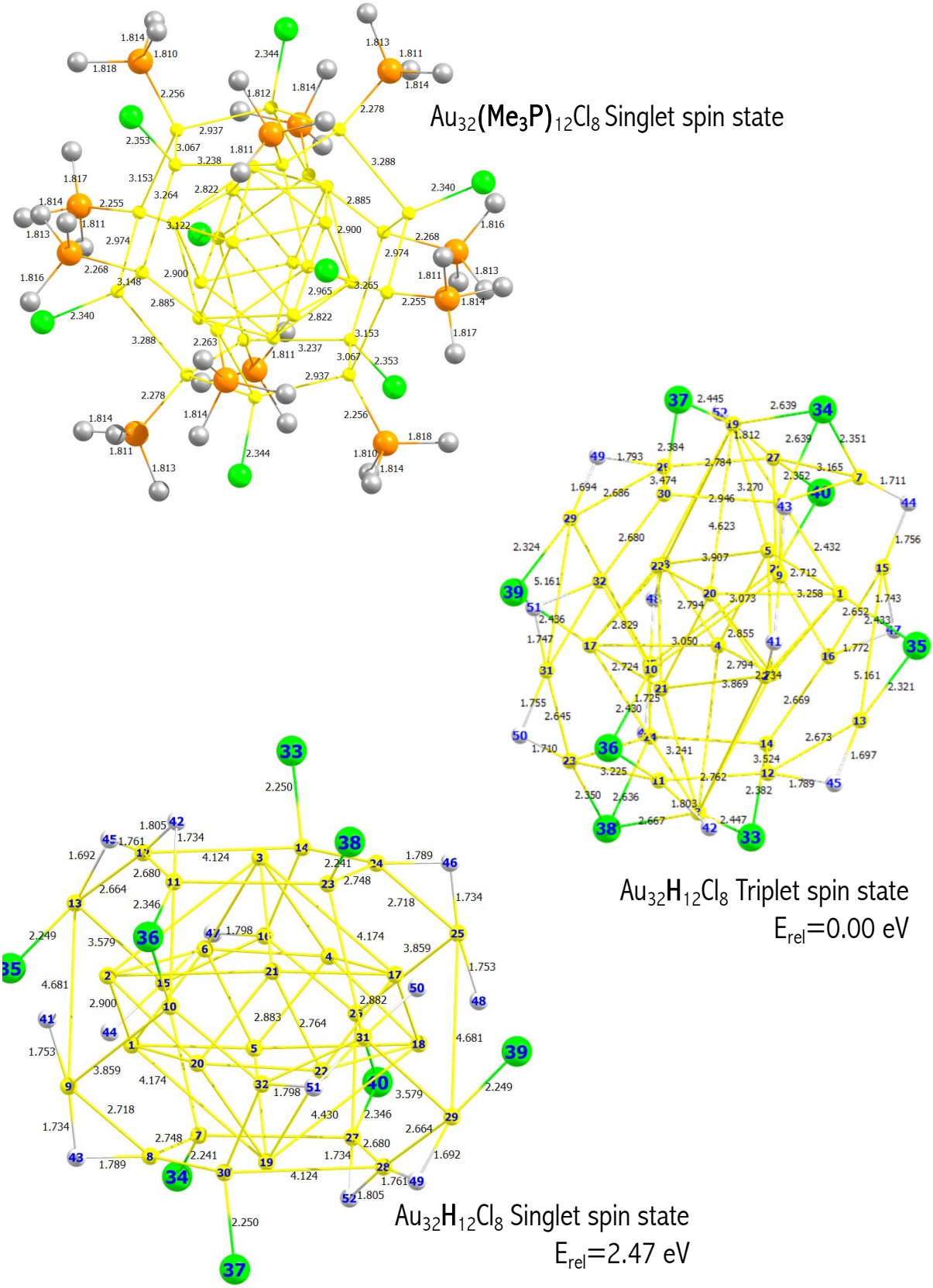


Figure S 5 The PBEsol/6-31++G(d,p)+LanL2DZ structures of $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ (top), $Au_{32}\mathbf{H}_{12}Cl_{12}$ triplet spin state (middle), and $Au_{32}\mathbf{H}_{12}Cl_{12}$ singlet spin state (bottom) isolated clusters with representative bond lengths (in Å). For the $Au_{32}(\mathbf{Me_3P})_{12}Cl_8$ structure, hydrogen atoms are omitted for clarity. Atoms are coloured yellow (Au), grey (C), green (Cl), white (H), and orange (P). For the $Au_{32}\mathbf{H}_{12}Cl_8$ structures, the PBE0-D3 adiabatic relative energies (E_{rel} in eV) are provided.

5. Topological analysis of the bonding

We decided to incorporate into our analysis a delocalized view of electrons in molecules that is at variance with the chemically intuitive notion of localized bonds and lone pairs inherited from Lewis. To introduce a localized view of electrons within studied systems, we used the Electron Localization Function (ELF) [10] and the Quantum Theory of Atoms in Molecules (QTAIM). [11] The ELF is a mathematical function that relates to the probability of finding an electron pair in the vicinity of a particular point in space. It is normalized so that $0 \leq ELF \leq 1$ and increases with the increasing probability of finding a localized electron pair. The QTAIM is a topological analysis of the properties of the electron density (ρ), its gradient ($\nabla\rho$), and its Laplacian ($\nabla^2\rho$) in the three-dimensional Euclidean space. In the QTAIM approach, atoms emerge as non-overlapping regions of space (atomic basins) defined by their kinetic energies, and separated by interatomic surfaces. [11] In general, bonded atoms are connected by a bond path crossing a bond critical point (BCP), i.e. a saddle point of the electron density. [12] Although there is no strict equivalence between BCPs and chemical bonds, their absence can be used as a metric to determine a lack of covalent bond. [12]

We used the VASP package (Rev.6.3.2) [3-6] and Critic2 software (Rev.3) [13] to estimate ELF and BCP values. The obtained results were visualized with the VESTA software.

6. Electron affinity and ionization energy of isolated ligands

The adiabatic electron affinity (AEA) of ligands was estimated as the electronic energy differences between the neutral (E_{neu}) and anion (E_{neu}) at each equilibrium geometry ($r_{e,0}$ and $r_{e,-}$, respectively, Equation S 1). We calculated the adiabatic ionization energy (AIE) by subtracting the total electronic energies of the cation (E_{cat}) and neutral (E_{neu}) at each equilibrium geometry ($r_{e,+}$ and $r_{e,-}$, respectively, Equation S 2). The $AEA^{CCSD(T)}$ and $AIE^{CCSD(T)}$ values were obtained at the CCSD(T)/6-311++G(3df,3pd) level at the equilibrium geometries optimized at the MP2/6-311++G(d,p) theory level. The $AIE^{PBE0\text{-}D3}$, $VEA^{PBE0\text{-}D3}$, and $AEA^{PBE0\text{-}D3}$ were calculated at the PBE0-D3/6-31++G(d,p) theory level.

$$AEA = E_{neu}(r_{e,0}) - E_{an}(r_{e,-}) \qquad \textit{Equation S 1}$$

$$AIE = E_{cat}(r_{e,+}) - E_{neu}(r_{e,0}) \qquad \textit{Equation S 2}$$

Table S 3 Adiabatic ionization energy (AIE) of ligands obtained at the PBE0-D3/6-31+G(d,p) ($AIE^{PBE0\text{-}D3}$ in eV) and CCSD(T)/6-311+G(3df,3pd) ($AIE^{CCSD(T)}$ in eV) levels. The PBE0-D3 vertical electron affinity ($VEA^{PBE0\text{-}D3}$ in eV), adiabatic electron affinity (AEA, obtained at the PBE0-D3/6-31+G(d,p) ($VEA^{PBE0\text{-}D3}$ in eV) and CCSD(T)/6-311+G(3df,3pd) ($VEA^{CCSD(T)}$ in eV) theory levels). Experimental values of vertical ionization energy (VIE^{exp}) and electron affinity (EA^{exp}) are also provided for comparison. [14]

Ligand	$AIE^{PBE0\text{-}D3}$	$AIE^{CCSD(T)}$	$AIE^{exp\ 14}$	$VIE^{exp\ 14}$	$VEA^{PBE0\text{-}D3}$	$AEA^{PBE0\text{-}D3}$	$AEA^{CCSD(T)}$	EA^{exp}
H	13.63	13.60	13.60	-	0.60	0.60	0.65	0.755
PH_3	9.70	9.75	9.87±0.01	10.59±0.05	-0.70	-0.69	-0.83	-
PMe_3	7.67	7.82	8.1±0.1	8.6±0.1	-0.67	-0.66	-0.76	-
PEt_3	7.38	7.56	7.6	8.31	-0.62	-0.63	-0.93	-
$^{n}PPr_3$	7.27	7.31	-	-	-0.57	-065	-0.99	-
$^{n}Bu_3P$	7.20	7.25	7.5	8.00	-0.54	-0.79	-0.79	-

In Figure S 6a we shown AIE and AEA values of ligands obtained at the CCSD(T) level of theory. The only issue we want to raise considering the comparison of the CCSD(T) values to PBE0-D3 ones (provided in *Table S 3*) is the observation that the AIE and AEA values are underestimated at the PBE0-D3 level of theory (with respect to CCSD(T) values).

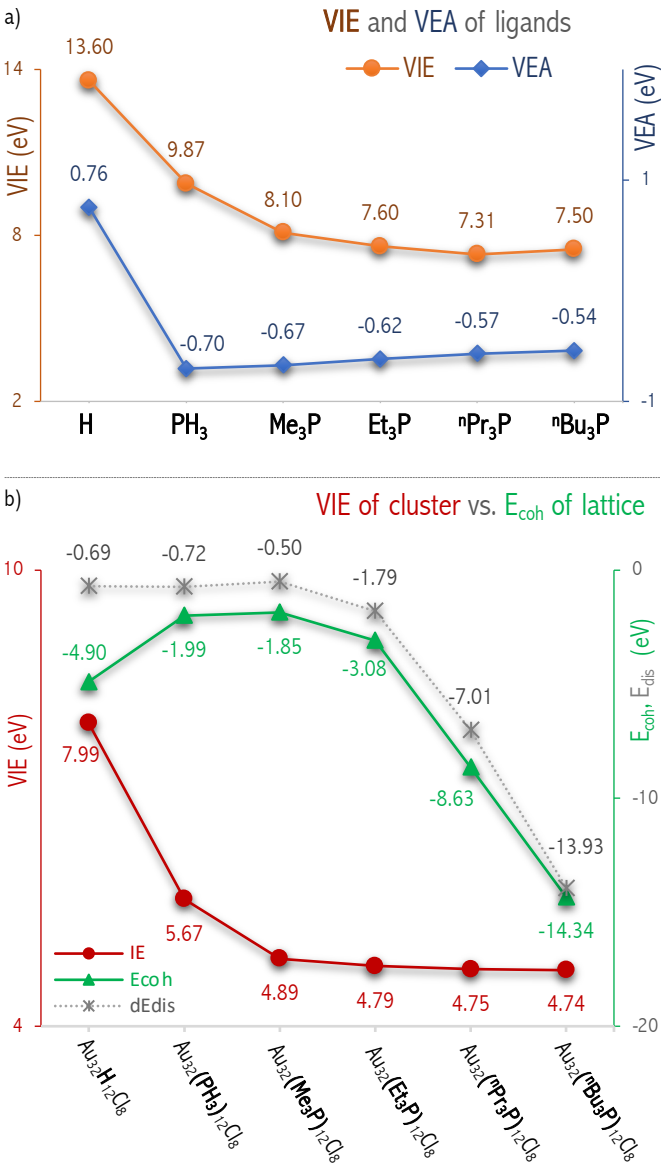


Figure S 6 a) The adiabatic electron affinity (AEA, blue diamonds) and adiabatic ionization energy (AIE, orange circles) values of ligands as obtained from CCSD(T)/6-311++G(3df,3pd) method at the equilibrium geometries optimized at the MP2/6-311++G(d,p). b) The PBE0-D3 ionization energy of cluster (IE in eV) and PBE0-D3 cohesive energy of $Au_{32}(\boldsymbol{R_3P})_{12}Cl_8$ lattice (E_{coh} in eV).

7. Vertical ionization energy (VIE) and vertical electron affinity (VEA) values of singlet spin state gold clusters

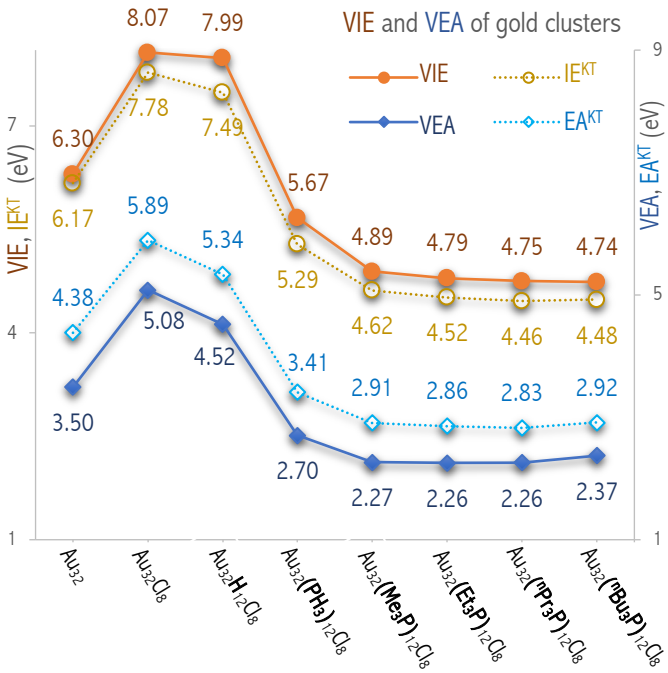
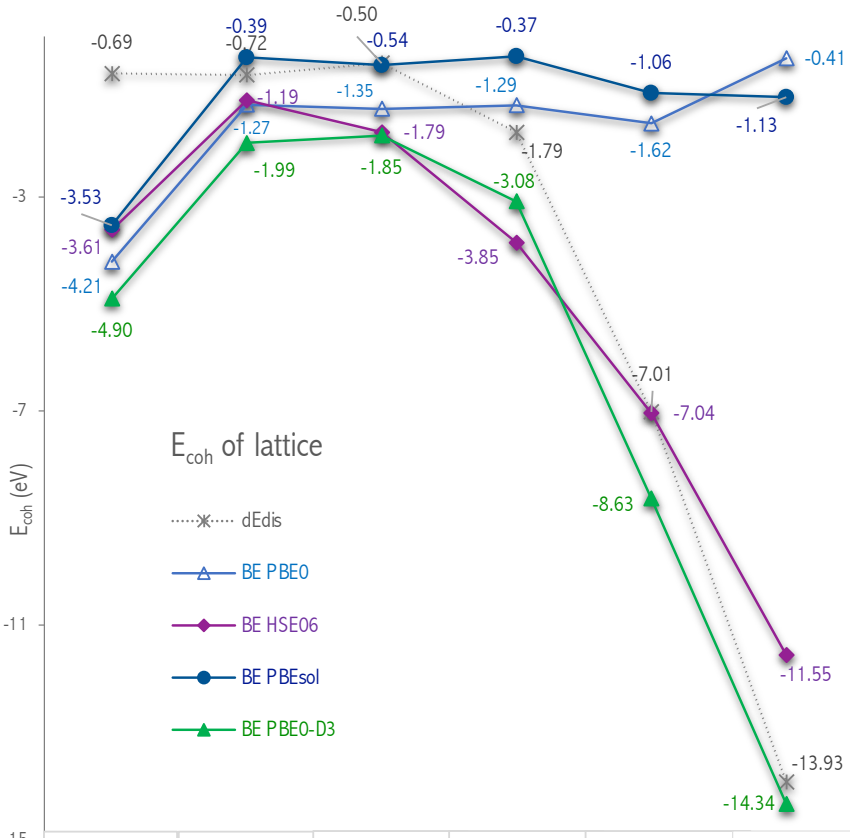


Figure S 7 The vertical ionization energy (VIE) and vertical electron affinity (VEA) values of gold clusters as obtained from the PBE0-D3/6-31++G(d,p)+LanL2DZ method. The energies have been estimated at the singlet spin state equilibrium neutral geometries for all systems.

8. Cohesive energy of lattice

Figure S2 shows the cohesive energy of studied lattices obtained at the PBEsol (navy circles), PBE0 (orange circles), PBE0-D3 (green triangles), and HSE06-D3 (purple diamonds) levels of theory. Dispersion energy (E_{dis}, grey stars in Figure S 8) has been obtained as a difference between cohesive energies obtained at the PBE0-D3 and PBE0 theory levels ($E_{dis}=E_{coh}^{PBE0\text{-}D3} - E_{coh}^{PBE0}$).



	$Au_{32}H_{12}Cl_8$	$Au_{32}(PH_3)_{12}Cl_8$	$Au_{32}(Me_3P)_{12}Cl_8$	$Au_{32}(Et_3P)_{12}Cl_8$	$Au_{32}(^nPr_3P)_{12}Cl_8$	$Au_{32}(^nBu_3P)_{12}Cl_8$
dEdis	-0.69	-0.72	-0.50	-1.79	-7.01	-13.93
BE PBE0	-4.21	-1.27	-1.35	-1.29	-1.62	-0.41
BE HSE06	-3.61	-1.19	-1.79	-3.85	-7.04	-11.55
BE PBEsol	-3.53	-0.39	-0.54	-0.37	-1.06	-1.13
BE PBE0-D3	-4.90	-1.99	-1.85	-3.08	-8.63	-14.34

Figure S 8 a) The cohesive energy (E_{coh}) of superatomic lattice obtained at the PBEsol (navy circles), PBE0 (blue triangles), PBE0-D3 (green triangles), and HSE06-D3 (purple diamonds) levels of theory. Dispersion energy (E_{dis}, grey stars) has been obtained as a difference between cohesive energies obtained at the PBE0-D3 and PBE0 levels. The isolated gold clusters at the equilibrium geometry of singlet spin state.

9. Lattice parameters and atomic coordinates of the ligand-protected gold clusters

POSCAR FILE OF THE $Au_{32}(^NBu_3P)_{12}Cl_8$ ASSEMBLY SYSTEM 17

POSCAR FILE OF THE $Au_{32}(^NPr_3P)_{12}Cl_8$ ASSEMBLY SYSTEM 41

POSCAR FILE OF THE $Au_{32}(Et_3P)_{12}Cl_8$ ASSEMBLY SYSTEM 60

POSCAR FILE OF THE $Au_{32}(Me_3P)_{12}Cl_8$ ASSEMBLY SYSTEM..... 75

POSCAR FILE OF THE $Au_{32}(P_3H)_{12}Cl_8$ ASSEMBLY SYSTEM 84

POSCAR FILE OF THE $Au_{32}H_{12}Cl_8$ ASSEMBLY SYSTEM..... 88

POSCAR file of the $Au_{32}(^{n}Bu_3P)_{12}Cl_8$ assembly system

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0.300369	-0.719782	-0.662953	C
0.734728	-0.228995	-1.358231	C
0.265272	-0.771005	-0.641769	C
0.719922	-0.141682	-1.389996	C
0.280078	-0.858318	-0.610004	C
0.602797	-0.126957	-1.208161	C
0.397203	-0.873043	-0.791839	C
0.599591	-0.04746	-1.205117	C
0.400409	-0.95254	-0.794883	C
0.638167	-0.037072	-1.184188	C
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0.678803	-0.028307	-1.248531	C
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0.565715	-0.097762	-1.33981	C
0.434285	-0.902238	-0.66019	C
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0.399678	-0.862481	-0.61415	C
0.60601	-0.093079	-1.475492	C
0.39399	-0.906921	-0.524508	C
0.61968	-0.010742	-1.508366	C
0.38032	-0.989258	-0.491634	C

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0.545976	-0.013497	-0.778884	C
0.509064	-0.103496	-1.193294	C
0.490936	-0.896504	-0.806706	C
0.501142	-0.013708	-1.229657	C
0.498858	-0.986292	-0.770343	C
0.445283	-0.897948	-1.247312	C
0.554717	-0.102052	-0.752688	C
0.305512	-0.261949	-1.085584	C
0.694488	-0.738051	-0.914416	C
0.324741	-0.199451	-1.272095	C
0.675259	-0.800549	-0.727905	C
0.324421	-0.31022	-1.1343	C
0.675579	-0.68978	-0.8657	C
0.349866	-0.267082	-1.218103	C
0.650134	-0.732918	-0.781897	C
0.355501	-0.126478	-1.139639	C
0.644499	-0.873522	-0.860361	C
0.318701	-0.062895	-1.156226	C
0.681299	-0.937105	-0.843774	C
0.333363	-0.982848	-1.218117	C
0.666637	-0.017152	-0.781883	C
0.352473	-0.980541	-1.300605	C
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0.302151	-0.082035	-0.858761	C
0.697849	-0.917965	-1.141239	C
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0.452258	-0.09175	-0.991173	C
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0.402205	-0.965581	-1.033399	C
0.597795	-0.034419	-0.966601	C
0.394611	-0.261651	-0.763492	C
0.605389	-0.738349	-1.236508	C
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0.133792	-0.228665	-0.895068	H
0.795386	-0.691009	-1.078913	H
0.204614	-0.308991	-0.921087	H
0.841541	-0.646739	-1.098408	H
0.158459	-0.353261	-0.901592	H
0.788749	-0.54878	-1.172256	H
0.211251	-0.45122	-0.827744	H
0.836553	-0.56397	-1.239457	H
0.163447	-0.43603	-0.760543	H
0.790181	-0.607539	-1.22245	H
0.209819	-0.392461	-0.77755	H
0.903147	-0.73921	-1.31891	H
0.096853	-0.26079	-0.68109	H
0.900846	-0.814403	-1.346349	H
0.099154	-0.185597	-0.653651	H
0.830758	-0.678702	-1.346195	H
0.169242	-0.321298	-0.653805	H
0.82656	-0.756269	-1.369268	H
0.17344	-0.243731	-0.630732	H
0.890869	-0.717555	-1.481633	H
0.109131	-0.282445	-0.518367	H
0.894126	-0.638575	-1.460193	H
0.105874	-0.361425	-0.539807	H
0.856311	-0.593833	-1.570791	H
0.143689	-0.406167	-0.429209	H
0.817299	-0.660373	-1.505762	H
0.182701	-0.339627	-0.494238	H
0.821739	-0.579278	-1.487467	H
0.178261	-0.420722	-0.512533	H
0.499013	-0.530253	-0.60604	H
0.500987	-0.469747	-1.39396	H
0.515233	-0.613989	-0.526067	H
0.484767	-0.386011	-1.473933	H
0.59279	-0.589675	-0.598165	H
0.40721	-0.410325	-1.401835	H
0.574977	-0.502696	-0.672055	H

0.425023	-0.497304	-1.327945	H
0.556923	-0.539562	-1.49423	H
0.443077	-0.460438	-0.50577	H
0.536978	-0.452673	-0.565216	H
0.463022	-0.547327	-1.434784	H
0.602751	-0.433869	-1.537633	H
0.397249	-0.566131	-0.462367	H
0.632045	-0.506789	-1.570957	H
0.367955	-0.493211	-0.429043	H
0.611362	-0.416761	-0.63929	H
0.388638	-0.583239	-1.36071	H
0.571794	-0.754368	-0.641456	H
0.428206	-0.245632	-1.358544	H
0.600171	-0.687995	-0.637375	H
0.399829	-0.312005	-1.362625	H
0.538806	-0.802201	-1.499176	H
0.461194	-0.197799	-0.500824	H
0.556569	-0.726544	-1.489697	H
0.443431	-0.273456	-0.510303	H
0.615633	-0.851435	-1.539618	H
0.384367	-0.148565	-0.460382	H
0.631355	-0.780126	-1.520778	H
0.368645	-0.219874	-0.479222	H
0.628582	-0.912223	-1.403057	H
0.371418	-0.087777	-0.596943	H
0.590987	-0.840614	-1.377818	H
0.409013	-0.159386	-0.622182	H
0.573834	-0.910802	-1.396977	H
0.426166	-0.089198	-0.603023	H
0.457561	-0.63524	-0.643647	H
0.542439	-0.36476	-1.356353	H
0.484986	-0.730062	-0.624731	H
0.515014	-0.269938	-1.375269	H
0.452407	-0.654681	-0.503574	H
0.547593	-0.345319	-1.496426	H
0.47585	-0.752684	-0.481216	H
0.52415	-0.247316	-1.518784	H
0.394186	-0.681818	-0.539773	H
0.605814	-0.318182	-1.460227	H
0.416625	-0.77938	-0.521582	H
0.583375	-0.22062	-1.478418	H
0.35811	-0.775928	-0.405357	H
0.64189	-0.224072	-1.594643	H

0.407416	-0.809465	-1.377185	H
0.592584	-0.190535	-0.622815	H
0.385123	-0.711092	-0.395227	H
0.614877	-0.288908	-1.604773	H
0.701421	-0.532108	-0.883732	H
0.298579	-0.467892	-1.116268	H
0.718398	-0.461897	-0.864264	H
0.281602	-0.538103	-1.135736	H
0.663711	-0.496501	-0.735375	H
0.336289	-0.503499	-1.264625	H
0.64367	-0.562205	-0.755859	H
0.35633	-0.437795	-1.244141	H
0.71278	-0.644551	-0.755153	H
0.28722	-0.355449	-1.244847	H
0.735402	-0.5769	-0.741821	H
0.264598	-0.4231	-1.258179	H
0.713619	-0.693477	-1.612249	H
0.286381	-0.306523	-0.387751	H
0.684417	-0.604778	-1.608853	H
0.315583	-0.395222	-0.391147	H
0.660344	-0.671278	-1.622122	H
0.339656	-0.328722	-0.377878	H
0.713037	-0.344806	-0.993263	H
0.286963	-0.655194	-1.006737	H
0.705539	-0.417827	-1.021212	H
0.294461	-0.582173	-0.978788	H
0.651254	-0.258289	-1.052477	H
0.348746	-0.741711	-0.947523	H
0.643213	-0.334317	-1.073907	H
0.356787	-0.665683	-0.926093	H
0.715786	-0.326275	-1.163268	H
0.284214	-0.673725	-0.836732	H
0.681825	-0.238796	-1.194769	H
0.318175	-0.761204	-0.805231	H
0.753531	-0.204607	-1.211551	H
0.246469	-0.795393	-0.788449	H
0.716622	-0.178181	-1.137311	H
0.283378	-0.821819	-0.862689	H
0.752536	-0.264311	-1.109922	H
0.247464	-0.735689	-0.890078	H
0.614411	-0.301232	-0.897822	H
0.385589	-0.698768	-1.102178	H
0.614038	-0.379996	-0.803915	H

0.385962	-0.620004	-1.196085	H
0.690371	-0.360407	-0.817273	H
0.309629	-0.639593	-1.182727	H
0.689071	-0.278981	-0.909481	H
0.310929	-0.721019	-1.090519	H
0.627896	-0.293146	-0.750791	H
0.372104	-0.706854	-1.249209	H
0.628209	-0.211584	-0.842827	H
0.371791	-0.788416	-1.157173	H
0.666432	-0.186763	-0.762872	H
0.333568	-0.813237	-1.237128	H
0.701705	-0.272542	-0.757327	H
0.298295	-0.727458	-1.242673	H
0.702485	-0.189869	-0.850428	H
0.297515	-0.810131	-1.149572	H
0.639896	-0.439452	-1.373587	H
0.360104	-0.560548	-0.626413	H
0.658567	-0.346105	-1.410942	H
0.341433	-0.653895	-0.589058	H
0.734565	-0.408153	-1.445957	H
0.265435	-0.591847	-0.554043	H
0.713213	-0.498566	-1.412014	H
0.286787	-0.501434	-0.587986	H
0.668286	-0.434988	-1.511242	H
0.331714	-0.565012	-0.488758	H
0.689694	-0.34467	-1.546609	H
0.310306	-0.65533	-0.453391	H
0.726608	-0.415625	-1.633657	H
0.273392	-0.584375	-0.366343	H
0.763015	-0.407457	-1.586829	H
0.236985	-0.592543	-0.413171	H
0.741384	-0.498456	-1.551184	H
0.258616	-0.501544	-0.448816	H
0.732345	-0.524135	-1.300005	H
0.267655	-0.475865	-0.699995	H
0.712081	-0.537821	-1.199087	H
0.287919	-0.462179	-0.800913	H
0.653709	-0.60577	-1.181199	H
0.346291	-0.39423	-0.818801	H
0.65989	-0.576329	-1.283554	H
0.34011	-0.423671	-0.716446	H
0.687321	-0.719422	-1.205399	H
0.312679	-0.280578	-0.794601	H

0.728433	-0.681739	-1.195539	H
0.271567	-0.318261	-0.804461	H
0.752036	-0.720271	-1.310933	H
0.247964	-0.279729	-0.689067	H
0.711313	-0.652626	-1.354705	H
0.288687	-0.347374	-0.645295	H
0.754101	-0.617708	-1.344985	H
0.245899	-0.382292	-0.655015	H
0.72307	-0.387647	-1.247772	H
0.27693	-0.612353	-0.752228	H
0.74259	-0.380651	-1.346427	H
0.25741	-0.619349	-0.653573	H
0.687487	-0.262641	-1.390391	H
0.312513	-0.737359	-0.609609	H
0.672373	-0.268701	-1.29276	H
0.327627	-0.731299	-0.70724	H
0.761708	-0.241043	-1.402645	H
0.238292	-0.758957	-0.597355	H
0.746983	-0.24638	-1.305106	H
0.253017	-0.75362	-0.694894	H
0.745064	-0.105164	-1.402545	H
0.254936	-0.894836	-0.597455	H
0.709475	-0.121992	-1.445338	H
0.290525	-0.878008	-0.554662	H
0.692778	-0.128512	-1.346804	H
0.307222	-0.871488	-0.653196	H
0.605198	-0.174132	-1.149236	H
0.394802	-0.825868	-0.850764	H
0.63163	-0.135994	-1.251241	H
0.36837	-0.864006	-0.748759	H
0.571237	-0.043954	-1.158831	H
0.428763	-0.956046	-0.841169	H
0.595091	-0.998339	-1.261868	H
0.404909	-0.001661	-0.738132	H
0.631043	-0.984608	-1.170659	H
0.368957	-0.015392	-0.829341	H
0.642539	-0.087792	-1.128294	H
0.357461	-0.912208	-0.871706	H
0.705337	-0.019572	-1.230837	H
0.294663	-0.980428	-0.769163	H
0.688511	-0.080825	-1.261695	H
0.311489	-0.919175	-0.738305	H
0.675133	-0.977093	-1.304342	H

0.324867	-0.022907	-0.695658	H
0.571867	-0.036396	-1.358228	H
0.428133	-0.963604	-0.641772	H
0.534483	-0.096107	-1.350542	H
0.465517	-0.903893	-0.649458	H
0.592774	-0.198441	-1.3658	H
0.407226	-0.801559	-0.6342	H
0.63085	-0.14316	-1.370822	H
0.36915	-0.85684	-0.629178	H
0.629696	-0.12785	-1.504496	H
0.370304	-0.87215	-0.495504	H
0.57602	-0.089408	-1.491365	H
0.42398	-0.910592	-0.508635	H
0.624797	-0.981505	-1.573392	H
0.375203	-0.018495	-0.426608	H
0.595437	-0.972871	-1.484553	H
0.404563	-0.027129	-0.515447	H
0.649405	-0.012244	-1.492921	H
0.350595	-0.987756	-0.507079	H
0.441251	-0.006066	-1.255503	H
0.558749	-0.993934	-0.744497	H
0.437235	-0.016901	-1.158464	H
0.562765	-0.983099	-0.841536	H
0.485366	-0.129364	-1.202856	H
0.514634	-0.870636	-0.797144	H
0.505253	-0.128242	-1.128354	H
0.494747	-0.871758	-0.871646	H
0.515054	-0.988413	-1.201636	H
0.484946	-0.011587	-0.798364	H
0.51699	-0.988463	-1.293418	H
0.48301	-0.011537	-0.706582	H
0.411203	-0.878474	-1.242496	H
0.588797	-0.121526	-0.757504	H
0.456179	-0.87845	-1.210711	H
0.543821	-0.12155	-0.789289	H
0.461948	-0.866031	-1.30955	H
0.538052	-0.133969	-0.69045	H
0.287131	-0.30061	-1.027251	H
0.712869	-0.69939	-0.972749	H
0.283158	-0.21179	-1.112984	H
0.716842	-0.78821	-0.887016	H
0.344626	-0.170979	-1.332253	H
0.655374	-0.829021	-0.667747	H

0.297583	-0.219983	-1.277684	H
0.702417	-0.780017	-0.722316	H
0.311968	-0.153229	-1.249757	H
0.688032	-0.846771	-0.750243	H
0.297818	-0.335479	-1.136253	H
0.702182	-0.664521	-0.863747	H
0.344545	-0.361411	-1.101111	H
0.655455	-0.638589	-0.898889	H
0.363334	-0.310686	-1.243868	H
0.636666	-0.689314	-0.756132	H
0.37791	-0.245632	-1.21637	H
0.62209	-0.754368	-0.78363	H
0.378885	-0.107845	-1.122173	H
0.621115	-0.892155	-0.877827	H
0.373608	-0.137109	-1.19258	H
0.626392	-0.862891	-0.80742	H
0.30036	-0.057135	-1.100963	H
0.69964	-0.942865	-0.899037	H
0.295961	-0.080138	-1.176336	H
0.704039	-0.919862	-0.823664	H
0.305997	-0.937887	-1.219885	H
0.694003	-0.062113	-0.780115	H
0.356618	-0.966495	-1.198329	H
0.643382	-0.033505	-0.801671	H
0.362432	-0.921849	-1.343895	H
0.637568	-0.078151	-0.656105	H
0.380523	-0.02347	-1.301888	H
0.619477	-0.97653	-0.698112	H
0.329122	-0.994703	-1.321781	H
0.670878	-0.005297	-0.678219	H
0.277027	-0.167165	-1.001578	H
0.722973	-0.832835	-0.998422	H
0.29613	-0.256954	-0.931571	H
0.70387	-0.743046	-1.068429	H
0.339368	-0.103818	-0.99949	H
0.660632	-0.896182	-1.00051	H
0.347273	-0.192312	-0.916831	H
0.652727	-0.807688	-1.083169	H
0.268922	-0.172314	-0.850595	H
0.731078	-0.827686	-1.149405	H
0.264768	-0.082263	-0.933192	H
0.735232	-0.917737	-1.066808	H
0.275262	-0.059069	-0.822629	H

0.724738	-0.940931	-1.177371	H
0.322948	-0.122688	-0.819236	H
0.677052	-0.877312	-1.180764	H
0.320127	-0.031735	-0.903717	H
0.679873	-0.968265	-1.096283	H
0.468766	-0.979847	-1.086797	H
0.531234	-0.020153	-0.913203	H
0.458025	-0.980495	-0.991903	H
0.541975	-0.019505	-1.008097	H
0.390771	-0.11894	-0.908433	H
0.609229	-0.88106	-1.091567	H
0.427695	-0.097742	-0.871911	H
0.572305	-0.902258	-1.128089	H
0.485979	-0.112805	-0.99077	H
0.514021	-0.887195	-1.00923	H
0.44406	-0.114027	-1.028623	H
0.55594	-0.885973	-0.971377	H
0.400872	-0.90075	-1.061447	H
0.599128	-0.09925	-0.938553	H
0.389892	-0.984967	-1.068459	H
0.610108	-0.015033	-0.931541	H
0.380256	-0.981862	-0.974398	H
0.619744	-0.018138	-1.025602	H
0.36633	-0.25761	-0.784611	H
0.63367	-0.74239	-1.215389	H
0.401916	-0.325228	-0.728201	H
0.598084	-0.674772	-1.271799	H
0.382094	-0.15024	-0.752518	H
0.617906	-0.84976	-1.247482	H
0.412933	-0.223657	-0.688646	H
0.587067	-0.776343	-1.311354	H
0.338015	-0.191682	-0.620986	H
0.661985	-0.808318	-1.379014	H
0.318582	-0.22807	-0.67286	H
0.681418	-0.77193	-1.32714	H
0.319577	-0.331232	-0.53672	H
0.680423	-0.668768	-1.46328	H
0.357902	-0.363484	-0.605847	H
0.642098	-0.636516	-1.394153	H
0.374465	-0.324111	-0.552637	H
0.625535	-0.675889	-1.447363	H
0.507988	-0.203373	-0.872062	H
0.492012	-0.796627	-1.127938	H

0.473477	-0.198662	-0.783302	H
0.526523	-0.801338	-1.216698	H
0.476196	-0.355597	-0.730814	H
0.523804	-0.644403	-1.269186	H
0.519278	-0.34376	-0.813553	H
0.480722	-0.65624	-1.186447	H
0.554616	-0.274501	-0.76262	H
0.445384	-0.725499	-1.23738	H
0.548497	-0.37552	-0.701986	H
0.451503	-0.62448	-1.298014	H
0.528	-0.300104	-0.617967	H
0.472	-0.699896	-1.382033	H
0.489548	-0.238478	-0.671246	H
0.510452	-0.761522	-1.328754	H
0.48286	-0.340523	-0.613179	H
0.51714	-0.659477	-1.386821	H

POSCAR file of the $Au_{32}(^{n}Pr_3P)_{12}Cl_8$ assembly system

1				
-6.50777	-7.497128	31.163662		
-18.781919	0	0		
-8.389586	-16.973016	0		
Au	Cl	P	C	H
64	16	24	216	504
direct				
0.993413	-0.946175	-1.150125	Au	
0.93514	-0.876976	-1.051988	Au	
0.96106	-0.744938	-1.055756	Au	
0.97817	-0.781433	-1.210328	Au	
0.893542	-0.836065	-0.927895	Au	
0.907546	-0.919138	-1.153979	Au	
0.859859	-0.955318	-0.959627	Au	
0.932466	-0.040475	-1.019581	Au	
0.949969	-0.202814	-0.992296	Au	
0.958182	-0.061644	-1.160326	Au	
0.067519	-0.959681	-0.980478	Au	
0.049552	-0.797124	-1.007779	Au	
0.041852	-0.938322	-0.83995	Au	
0.973897	-0.148431	-1.900662	Au	
0.93664	-0.140764	-1.75294	Au	
0.882062	-0.121441	-1.866527	Au	
0.924513	-0.000709	-1.886098	Au	

0.025943	-0.852448	-0.099132	Au
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0.967376	-0.628453	-1.804704	H
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0.067204	-0.030379	-0.66274	H
0.100133	-0.96658	-0.662565	H
0.06301	-0.991259	-0.517499	H
0.028639	-0.054107	-0.516607	H

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0.076405	-0.714521	-0.786309	H
0.093813	-0.797424	-0.705513	H
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0.16962	-0.789805	-0.792547	H
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0.882176	-0.080112	-1.611557	H
0.852679	-0.220548	-1.447328	H
0.896133	-0.163725	-1.473573	H
0.846776	-0.038939	-1.498768	H
0.802182	-0.094648	-1.471872	H
0.907759	-0.329753	-1.619628	H
0.858843	-0.271136	-1.632161	H
0.885539	-0.36195	-1.468879	H
0.836591	-0.303465	-1.482269	H
0.817053	-0.393775	-1.531941	H
0.866442	-0.452564	-1.519275	H
0.970985	-0.288828	-1.581996	H
0.936394	-0.27074	-1.497726	H
0.995971	-0.154869	-1.646425	H
0.96008	-0.126069	-1.572087	H
0.033981	-0.165686	-0.543923	H
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0.117878	-0.919881	-0.38845	H
0.147369	-0.779395	-0.552636	H
0.103907	-0.83618	-0.526421	H
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0.659392	-0.784973	-1.40842	H
0.31723	-0.235616	-0.653936	H
0.682775	-0.76433	-1.346148	H
0.509002	-0.202596	-0.866115	H
0.491006	-0.797439	-1.133861	H
0.474514	-0.195465	-0.776374	H
0.525487	-0.804591	-1.2236	H
0.477443	-0.351206	-0.71196	H
0.522533	-0.648828	-1.288044	H
0.516191	-0.347893	-0.800372	H
0.483778	-0.652158	-1.199631	H
0.562776	-0.271762	-0.775149	H
0.437223	-0.728333	-1.224846	H
0.552929	-0.367123	-0.693471	H
0.447053	-0.632986	-1.306558	H
0.652128	-0.968223	-1.212403	H
0.646102	-0.067739	-1.136997	H
0.347869	-0.031763	-0.787584	H
0.353895	-0.93225	-0.862989	H
0.363247	-0.989763	-1.294012	H
0.317394	-0.081361	-0.876301	H
0.448535	-0.917723	-1.253422	H

0.414237	-0.980146	-1.031555	H
0.524342	-0.279656	-0.683624	H
0.350866	-0.310704	-0.594584	H
0.597755	-0.465735	-1.578111	H
0.602689	-0.871144	-1.43813	H
0.399651	-0.758616	-0.411564	H
0.382139	-0.980131	-0.494938	H
0.551402	-0.082392	-0.746407	H
0.320957	-0.949818	-0.764254	H
0.31422	-0.779891	-1.182316	H
0.268776	-0.753082	-0.859132	H
0.316038	-0.361487	-0.353556	H
0.397333	-0.128776	-0.56184	H
0.402592	-0.534871	-0.421965	H
0.60027	-0.241062	-1.588516	H
0.72032	-0.430634	-1.568296	H
0.649142	-0.68918	-1.405455	H
0.738094	-0.655781	-1.29633	H
0.722941	-0.156101	-1.388769	H
0.679039	-0.05017	-1.235732	H
0.617869	-0.019842	-1.505077	H
0.685782	-0.220122	-0.817657	H
0.731193	-0.246819	-1.140745	H
0.684639	-0.638081	-1.646618	H
0.585763	-0.019784	-0.968413	H
0.475661	-0.720469	-1.316346	H
0.68262	-0.918614	-1.123678	H
0.636795	-0.010182	-0.705975	H
0.681738	-0.807158	-0.745697	H
0.279705	-0.569273	-0.431724	H
0.261903	-0.34417	-0.703692	H
0.277072	-0.843857	-0.61124	H
0.318309	-0.192793	-1.254312	H

POSCAR file of the $Au_{32}(Et_3P)_{12}Cl_8$ assembly system

1				
6.599518	7.269905	31.147601		
18.833293	0	0		
8.445458	17.108358	0		
Au	Cl	P	C	H
64	16	24	144	360
direct				

0.992997	0.054027	0.850593	Au
0.935597	0.123488	0.948525	Au
0.960648	0.254343	0.946597	Au
0.977326	0.218096	0.791442	Au
0.89509	0.160882	0.074517	Au
0.906553	0.080707	0.850063	Au
0.860443	0.04608	0.037282	Au
0.93279	0.959821	0.980119	Au
0.949817	0.797565	0.007671	Au
0.957291	0.939251	0.840704	Au
0.067216	0.040147	0.019905	Au
0.050182	0.202439	0.99233	Au
0.042708	0.06075	0.159295	Au
0.974307	0.85186	0.098472	Au
0.937044	0.860558	0.244178	Au
0.883014	0.879837	0.130507	Au
0.925231	0.999499	0.1121	Au
0.025678	0.148051	0.90162	Au
0.062932	0.139586	0.755993	Au
0.116983	0.120141	0.869491	Au
0.074754	0.000502	0.887867	Au
0.017974	0.888455	0.93636	Au
0.054282	0.970232	0.775395	Au
0.982029	0.111541	0.063701	Au
0.945381	0.029642	0.22453	Au
0.007	0.945966	0.149425	Au
0.064367	0.876392	0.051771	Au
0.03936	0.745684	0.053391	Au
0.022132	0.781732	0.209544	Au
0.104885	0.839199	0.925546	Au
0.093449	0.919298	0.149961	Au
0.139543	0.953912	0.962719	Au
0.572233	0.582897	0.946522	Au
0.427837	0.417175	0.053556	Au
0.489141	0.659286	0.951299	Au
0.51095	0.340638	0.048748	Au
0.427064	0.55204	0.08469	Au
0.572935	0.447976	0.915325	Au
0.475438	0.408719	0.165594	Au
0.524509	0.591395	0.834394	Au
0.562285	0.427183	0.074695	Au
0.437724	0.572837	0.925303	Au
0.511926	0.55702	0.096628	Au

0.488114	0.443008	0.903389	Au
0.640049	0.466079	0.962235	Au
0.359959	0.533924	0.037777	Au
0.612075	0.58596	0.797233	Au
0.387894	0.414038	0.202775	Au
0.558199	0.721049	0.816083	Au
0.441815	0.27893	0.183913	Au
0.462819	0.723021	0.813606	Au
0.53688	0.277442	0.186866	Au
0.401372	0.695334	0.96847	Au
0.598638	0.304641	0.031582	Au
0.450339	0.682308	0.091543	Au
0.549669	0.317691	0.908453	Au
0.545515	0.702827	0.00177	Au
0.454572	0.29719	0.998406	Au
0.441418	0.525067	0.22654	Au
0.558584	0.474943	0.773473	Au
0.599009	0.536124	0.089248	Au
0.401028	0.463892	0.910793	Au
0.540146	0.429632	0.22346	Au
0.459903	0.570302	0.776568	Au
0.788344	0.085751	0.032583	Cl
0.959301	0.33232	0.6828	Cl
0.921108	0.688873	0.013503	Cl
0.078929	0.311091	0.986503	Cl
0.079353	0.950433	0.65609	Cl
0.920651	0.049595	0.343842	Cl
0.211631	0.914152	0.967434	Cl
0.040642	0.66752	0.31766	Cl
0.420532	0.520493	0.357161	Cl
0.579473	0.479509	0.642842	Cl
0.715389	0.457535	0.942715	Cl
0.284629	0.542396	0.057263	Cl
0.570746	0.80963	0.005958	Cl
0.42934	0.190434	0.994117	Cl
0.450824	0.834453	0.697881	Cl
0.549135	0.165642	0.302112	Cl
0.836929	0.196911	0.155174	P
0.972879	0.383577	0.868353	P
0.855178	0.164358	0.785852	P
0.958017	0.864585	0.774025	P
0.041984	0.135431	0.225959	P
0.909896	0.797293	0.377018	P

0.089969	0.202848	0.623022	P
0.163025	0.803149	0.844806	P
0.027163	0.616468	0.131611	P
0.144826	0.835611	0.214134	P
0.833348	0.798584	0.154014	P
0.166659	0.201409	0.845982	P
0.528371	0.36127	0.359711	P
0.471649	0.638719	0.640324	P
0.656631	0.584431	0.091155	P
0.343425	0.415568	0.908851	P
0.675017	0.570297	0.713409	P
0.324957	0.42965	0.286569	P
0.560143	0.854936	0.765792	P
0.439883	0.145046	0.234215	P
0.342912	0.780996	0.940393	P
0.657076	0.218935	0.059676	P
0.438395	0.766435	0.152483	P
0.561611	0.233573	0.847495	P
0.797916	0.122577	0.210645	C
0.816479	0.042892	0.265079	C
0.85057	0.21804	0.230053	C
0.812923	0.244071	0.284912	C
0.805517	0.285459	0.099237	C
0.83128	0.357567	0.049222	C
0.978592	0.437851	0.923417	C
0.93936	0.437356	0.990219	C
0.930078	0.437442	0.81546	C
0.932859	0.526085	0.764119	C
0.024065	0.38827	0.79556	C
0.041616	0.469218	0.740867	C
0.814026	0.112462	0.784261	C
0.83275	0.054629	0.744901	C
0.823728	0.233176	0.828819	C
0.850464	0.28259	0.840768	C
0.879127	0.224248	0.680992	C
0.848045	0.279756	0.629968	C
0.999762	0.781738	0.795886	C
0.016664	0.744325	0.73557	C
0.968597	0.916886	0.664906	C
0.93644	0.988158	0.636448	C
0.906527	0.822163	0.8071	C
0.901613	0.767778	0.77078	C
0.000251	0.218302	0.204087	C

0.983343	0.255698	0.264419	C
0.031412	0.083123	0.335072	C
0.063572	0.011844	0.363499	C
0.093479	0.177836	0.192896	C
0.098389	0.232222	0.229221	C
0.871244	0.861394	0.419215	C
0.863727	0.838501	0.50886	C
0.884309	0.708797	0.400873	C
0.867755	0.655962	0.488962	C
0.952616	0.761449	0.431508	C
0.980164	0.82725	0.411211	C
0.12865	0.138735	0.580848	C
0.136216	0.161532	0.49121	C
0.115601	0.291345	0.599037	C
0.132216	0.344068	0.510935	C
0.047261	0.238644	0.568529	C
0.01976	0.172767	0.588859	C
0.202057	0.87744	0.789309	C
0.183504	0.957129	0.734884	C
0.149405	0.781978	0.769927	C
0.187068	0.755928	0.715098	C
0.194448	0.714602	0.900701	C
0.168692	0.642486	0.950717	C
0.021433	0.562162	0.076597	C
0.06067	0.562595	0.00982	C
0.069951	0.562612	0.184527	C
0.067147	0.473978	0.23588	C
0.975993	0.611872	0.204384	C
0.95838	0.53096	0.259027	C
0.185984	0.887534	0.21567	C
0.167275	0.945376	0.255022	C
0.176265	0.766801	0.171141	C
0.149509	0.717384	0.159229	C
0.120903	0.775731	0.318999	C
0.152011	0.720252	0.369992	C
0.848741	0.69238	0.204013	C
0.817053	0.636487	0.216292	C
0.781288	0.818188	0.21456	C
0.783347	0.803768	0.298494	C
0.82106	0.809286	0.062141	C
0.812806	0.895035	0.00442	C
0.151268	0.307616	0.79599	C
0.182958	0.36351	0.783699	C

0.218722	0.181826	0.785418	C
0.216662	0.196267	0.701482	C
0.178957	0.190689	0.937851	C
0.187208	0.104931	0.995562	C
0.522845	0.421491	0.415487	C
0.477189	0.578522	0.584511	C
0.562893	0.463613	0.392855	C
0.43715	0.536397	0.607134	C
0.571769	0.28405	0.389198	C
0.428249	0.715934	0.610836	C
0.568382	0.234567	0.478639	C
0.431628	0.76538	0.52139	C
0.478392	0.312999	0.396208	C
0.521631	0.686983	0.603813	C
0.456009	0.288698	0.484408	C
0.544006	0.711231	0.515611	C
0.692692	0.507778	0.14904	C
0.307356	0.492211	0.850977	C
0.671082	0.462893	0.236601	C
0.328942	0.537049	0.763399	C
0.692537	0.631352	0.993483	C
0.307518	0.36864	0.006508	C
0.670108	0.694809	0.929922	C
0.329948	0.305178	0.070053	C
0.640051	0.657008	0.135585	C
0.359998	0.343004	0.864412	C
0.675944	0.691314	0.143622	C
0.324107	0.308679	0.856385	C
0.667538	0.592342	0.614138	C
0.332445	0.407603	0.385834	C
0.70667	0.57394	0.556319	C
0.29331	0.426007	0.443648	C
0.703587	0.47164	0.747032	C
0.296409	0.52833	0.252934	C
0.677748	0.405727	0.761569	C
0.322266	0.594241	0.238329	C
0.715184	0.634609	0.696697	C
0.284807	0.365322	0.303264	C
0.698727	0.722018	0.667898	C
0.301267	0.277906	0.332115	C
0.604892	0.879171	0.788444	C
0.395127	0.120814	0.211568	C
0.611228	0.966327	0.760049	C

0.388804	0.033649	0.239962	C
0.565586	0.904703	0.657298	C
0.43444	0.095276	0.342706	C
0.602628	0.866882	0.611795	C
0.397383	0.133086	0.388205	C
0.50971	0.899152	0.808317	C
0.490315	0.100822	0.191673	C
0.501102	0.98934	0.774556	C
0.498925	0.01063	0.225434	C
0.307025	0.743713	0.909296	C
0.692971	0.256204	0.090774	C
0.329572	0.710742	0.846751	C
0.670431	0.289166	0.15332	C
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0.641068	0.124075	0.141649	C
0.322653	0.939046	0.83245	C
0.677341	0.060888	0.167565	C
0.307757	0.803886	0.022538	C
0.692216	0.196109	0.977467	C
0.330728	0.840444	0.055721	C
0.669221	0.159581	0.944286	C
0.426486	0.872746	0.094935	C
0.573514	0.127256	0.905024	C
0.453435	0.903756	0.009361	C
0.546588	0.096246	0.990611	C
0.394194	0.738209	0.241466	C
0.605817	0.261779	0.758517	C
0.385357	0.78712	0.290695	C
0.614645	0.212866	0.709291	C
0.485539	0.76321	0.187123	C
0.51446	0.236845	0.812857	C
0.503578	0.679574	0.234158	C
0.496457	0.320519	0.765802	C
0.770075	0.14761	0.244557	H
0.786938	0.116118	0.164138	H
0.84281	0.017008	0.229575	H
0.829714	0.048008	0.309562	H
0.869074	0.163773	0.264587	H
0.873863	0.263573	0.195957	H
0.789591	0.198816	0.31904	H
0.795607	0.300204	0.251286	H
0.793605	0.268673	0.060499	H
0.776987	0.297601	0.141928	H

0.842044	0.377178	0.087074	H
0.860267	0.343458	0.008743	H
0.007513	0.408086	0.947563	H
0.985749	0.499304	0.880684	H
0.932764	0.375809	0.032957	H
0.910362	0.466607	0.966763	H
0.929896	0.405195	0.779091	H
0.900014	0.425798	0.862514	H
0.960881	0.537745	0.713052	H
0.934928	0.558492	0.798864	H
0.046046	0.348364	0.834386	H
0.020357	0.356609	0.761129	H
0.076659	0.464535	0.73366	H
0.027901	0.514774	0.764635	H
0.797742	0.081296	0.847816	H
0.790036	0.157301	0.753948	H
0.857732	0.012315	0.774215	H
0.847869	0.08565	0.680783	H
0.801481	0.271045	0.789739	H
0.804124	0.195294	0.887165	H
0.872663	0.316921	0.784648	H
0.870222	0.244079	0.884426	H
0.903075	0.257399	0.682517	H
0.898039	0.181621	0.65603	H
0.829682	0.323311	0.653889	H
0.82487	0.247365	0.625738	H
0.026108	0.806297	0.801402	H
0.986171	0.738466	0.85695	H
0.033297	0.78715	0.677363	H
0.991157	0.722332	0.725137	H
0.0016	0.935111	0.646576	H
0.969173	0.87402	0.639504	H
0.936008	0.030159	0.662677	H
0.90354	0.970387	0.653947	H
0.902004	0.790329	0.873097	H
0.882055	0.873452	0.796153	H
0.923331	0.713039	0.78807	H
0.908136	0.796768	0.704658	H
0.973904	0.193764	0.198551	H
0.01385	0.26158	0.143033	H
0.966709	0.212861	0.32262	H
0.008843	0.277695	0.274864	H
0.998409	0.064898	0.353415	H

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0.063994	0.96986	0.337257	H
0.096474	0.029603	0.346	H
0.098008	0.209678	0.126896	H
0.11795	0.126545	0.203852	H
0.076668	0.28696	0.211935	H
0.091865	0.20323	0.295342	H
0.841201	0.866101	0.401146	H
0.883453	0.921024	0.385222	H
0.851201	0.77986	0.546267	H
0.893636	0.837816	0.525019	H
0.908871	0.675445	0.370578	H
0.85838	0.73075	0.367845	H
0.893342	0.634533	0.522438	H
0.841543	0.687167	0.51878	H
0.972422	0.714491	0.41353	H
0.938056	0.733573	0.496473	H
0.996922	0.849582	0.347198	H
0.961162	0.878671	0.421617	H
0.158672	0.134065	0.598966	H
0.116451	0.079096	0.614871	H
0.148747	0.220165	0.453767	H
0.106318	0.162185	0.475033	H
0.091076	0.324793	0.629271	H
0.141521	0.26934	0.632097	H
0.106656	0.365514	0.477394	H
0.158423	0.312762	0.481221	H
0.027426	0.285587	0.586497	H
0.061812	0.266517	0.503556	H
0.003007	0.150438	0.652874	H
0.038785	0.121359	0.578461	H
0.229878	0.852381	0.755382	H
0.213066	0.883884	0.83579	H
0.157184	0.983037	0.770378	H
0.170259	0.95201	0.690414	H
0.13091	0.836234	0.735354	H
0.126117	0.736438	0.804009	H
0.210403	0.801179	0.680962	H
0.204385	0.699802	0.748739	H
0.206374	0.731367	0.939439	H
0.22297	0.702476	0.85799	H
0.157934	0.622868	0.912866	H
0.139704	0.656588	0.991199	H

0.992521	0.591923	0.052423	H
0.014275	0.500718	0.119356	H
0.067277	0.624124	0.967028	H
0.089672	0.533362	0.03327	H
0.070131	0.594867	0.220885	H
0.100023	0.574227	0.137488	H
0.039105	0.462347	0.286914	H
0.065085	0.441574	0.201124	H
0.954023	0.651896	0.165588	H
0.979766	0.643439	0.238855	H
0.923363	0.535678	0.265921	H
0.972182	0.48532	0.235404	H
0.202253	0.918691	0.152107	H
0.209984	0.842703	0.24596	H
0.142291	0.987687	0.225716	H
0.152162	0.914362	0.319142	H
0.198519	0.728931	0.210199	H
0.195852	0.804681	0.112777	H
0.127315	0.683068	0.215368	H
0.129742	0.755881	0.115583	H
0.096951	0.742551	0.317524	H
0.101997	0.818356	0.343968	H
0.17037	0.676694	0.346068	H
0.175189	0.752666	0.374179	H
0.879892	0.682463	0.165342	H
0.85541	0.68291	0.26123	H
0.813993	0.641133	0.15838	H
0.78479	0.648353	0.250193	H
0.770896	0.881052	0.180783	H
0.75807	0.781682	0.216373	H
0.791805	0.74048	0.334203	H
0.807706	0.83869	0.295453	H
0.849043	0.778617	0.034343	H
0.793135	0.775028	0.080426	H
0.841793	0.927336	0.982611	H
0.78686	0.928579	0.032088	H
0.12012	0.317535	0.834665	H
0.144595	0.317087	0.738776	H
0.186029	0.358859	0.841605	H
0.215217	0.351649	0.749782	H
0.229118	0.11896	0.81918	H
0.241936	0.218331	0.783615	H
0.208187	0.259551	0.66579	H

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0.150974	0.221353	0.965659	H
0.206882	0.224948	0.919573	H
0.15822	0.072637	0.017367	H
0.213154	0.071397	0.96788	H
0.175738	0.746497	0.671003	H
0.208464	0.999416	0.702095	H
0.188161	0.5923	0.98732	H
0.055686	0.530711	0.976886	H
0.09604	0.448151	0.260485	H
0.964583	0.5083	0.319335	H
0.855121	0.603113	0.494699	H
0.828196	0.574268	0.250076	H
0.804001	0.897038	0.951918	H
0.752183	0.821181	0.331339	H
0.840482	0.882937	0.525441	H
0.004662	0.804479	0.447247	H
0.134309	0.686325	0.431587	H
0.1923	0.979415	0.250895	H
0.170594	0.675431	0.13568	H
0.959799	0.306554	0.242538	H
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0.055408	0.980227	0.429404	H
0.944607	0.019758	0.570541	H
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0.829366	0.324519	0.864338	H
0.903947	0.55189	0.739556	H
0.035243	0.491967	0.680676	H
0.944343	0.469205	0.023186	H
0.824269	0.253476	0.329006	H
0.791529	0.000582	0.297832	H
0.811813	0.407755	0.012619	H
0.159464	0.117046	0.474723	H
0.995249	0.19546	0.552851	H
0.144882	0.396901	0.505162	H
0.247827	0.178879	0.668619	H
0.196019	0.10292	0.048061	H
0.171813	0.425733	0.749921	H
0.494465	0.46417	0.401964	H
0.505573	0.535852	0.598038	H

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0.485076	0.617278	0.519665	H
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0.408937	0.578953	0.59308	H
0.57061	0.501714	0.327946	H
0.429433	0.498295	0.672043	H
0.572935	0.246055	0.3578	H
0.427087	0.753956	0.642204	H
0.601578	0.314762	0.36076	H
0.398441	0.685222	0.639292	H
0.540893	0.198063	0.50563	H
0.459111	0.801901	0.494363	H
0.564937	0.271519	0.511877	H
0.43507	0.728406	0.488178	H
0.45696	0.356197	0.358018	H
0.543063	0.64379	0.642003	H
0.486613	0.262301	0.378583	H
0.513424	0.737706	0.621397	H
0.446098	0.340936	0.499121	H
0.553915	0.658966	0.500943	H
0.476095	0.246005	0.525277	H
0.523922	0.753899	0.474731	H
0.70423	0.467721	0.117712	H
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0.720884	0.535981	0.142916	H
0.279166	0.463971	0.857156	H
0.66076	0.502039	0.268844	H
0.339252	0.497859	0.731199	H
0.642242	0.437358	0.241453	H
0.357788	0.562612	0.758469	H
0.717972	0.655107	0.002668	H
0.282087	0.344889	0.997307	H
0.707808	0.581759	0.975779	H
0.292246	0.418223	0.024226	H
0.652399	0.742908	0.947744	H
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0.646491	0.668782	0.918676	H
0.353559	0.331185	0.081332	H
0.61924	0.704117	0.09846	H
0.380804	0.295887	0.90154	H
0.618455	0.626765	0.194452	H
0.381592	0.373234	0.805543	H
0.696359	0.644911	0.181645	H

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0.696761	0.723564	0.084722	H
0.303293	0.276415	0.915281	H
0.640431	0.558965	0.62478	H
0.359547	0.440996	0.37518	H
0.655521	0.655762	0.589621	H
0.344469	0.344189	0.410347	H
0.734469	0.605171	0.545909	H
0.265514	0.394769	0.454057	H
0.716671	0.509732	0.578635	H
0.283309	0.49021	0.421341	H
0.734002	0.474114	0.701605	H
0.266001	0.525886	0.298372	H
0.712005	0.462479	0.802881	H
0.287973	0.537475	0.197106	H
0.648744	0.400933	0.810379	H
0.351259	0.599025	0.189497	H
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0.723732	0.612695	0.75524	H
0.276278	0.387199	0.244711	H
0.744319	0.623981	0.654155	H
0.255661	0.375955	0.34578	H
0.690915	0.744851	0.608728	H
0.309065	0.255105	0.391294	H
0.669152	0.730903	0.710344	H
0.330853	0.269004	0.2897	H
0.599965	0.848133	0.854597	H
0.400057	0.151848	0.145415	H
0.633686	0.847794	0.763685	H
0.366333	0.152181	0.236337	H
0.584915	0.995288	0.792082	H
0.415117	0.004691	0.207928	H
0.613253	0.000421	0.695136	H
0.386774	0.999551	0.304876	H
0.568781	0.968573	0.636888	H
0.431255	0.031406	0.363114	H
0.534496	0.899897	0.648026	H
0.465523	0.1001	0.351991	H
0.599141	0.802961	0.633778	H
0.400865	0.197004	0.366237	H
0.633914	0.87204	0.619627	H
0.366105	0.127917	0.380355	H

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0.514764	0.127503	0.200272	H
0.507681	0.872675	0.873653	H
0.492338	0.1273	0.12634	H
0.52039	0.017087	0.792771	H
0.479632	0.982889	0.207222	H
0.507491	0.016335	0.708484	H
0.492538	0.983633	0.291505	H
0.291066	0.695949	0.964722	H
0.708921	0.303971	0.035343	H
0.282031	0.79245	0.888856	H
0.717969	0.207468	0.111192	H
0.305834	0.691508	0.829101	H
0.694167	0.308409	0.170965	H
0.351738	0.658192	0.871641	H
0.648256	0.341711	0.128447	H
0.380986	0.896442	0.87851	H
0.619002	0.103485	0.121533	H
0.379507	0.861123	0.80839	H
0.620481	0.138789	0.191668	H
0.302412	0.954652	0.881768	H
0.697576	0.045307	0.118225	H
0.30121	0.919604	0.810311	H
0.698792	0.080331	0.189689	H
0.279501	0.842668	0.001546	H
0.720473	0.157301	0.998435	H
0.295937	0.746573	0.068774	H
0.704036	0.253427	0.93125	H
0.342183	0.898194	0.010185	H
0.65777	0.101823	0.989806	H
0.358929	0.800753	0.07545	H
0.641017	0.199283	0.924586	H
0.391906	0.882249	0.095632	H
0.608098	0.117738	0.904287	H
0.431465	0.904226	0.128504	H
0.56851	0.095791	0.871458	H
0.488151	0.890884	0.007584	H
0.511869	0.109111	0.992425	H
0.446275	0.875046	0.975346	H
0.553767	0.124937	0.024622	H
0.365818	0.74135	0.219371	H
0.634193	0.258619	0.780622	H
0.401564	0.674312	0.277867	H

0.598457	0.32568	0.722113	H
0.377429	0.850717	0.255421	H
0.622568	0.149268	0.744571	H
0.413076	0.782137	0.315067	H
0.586925	0.217858	0.68492	H
0.509796	0.794058	0.132299	H
0.490191	0.20603	0.867674	H
0.476455	0.799522	0.222587	H
0.523528	0.200544	0.777383	H
0.47932	0.64408	0.285399	H
0.520733	0.355982	0.714576	H
0.516027	0.647132	0.19509	H
0.48402	0.352967	0.804865	H
0.722872	0.758671	0.662286	H
0.697141	0.347987	0.779277	H
0.699234	0.591968	0.497623	H
0.573396	0.739476	0.50254	H
0.402488	0.806442	0.511477	H
0.441701	0.49898	0.574054	H
0.642027	0.234171	0.657726	H
0.469646	0.318249	0.742761	H
0.5533	0.031397	0.021397	H
0.662391	0.733997	0.171229	H
0.693631	0.721355	0.872827	H
0.693058	0.414082	0.268139	H
0.558348	0.501022	0.425938	H
0.426625	0.260456	0.497445	H
0.597517	0.193496	0.488546	H
0.467039	0.005683	0.796715	H
0.641248	0.971556	0.772263	H
0.603617	0.895498	0.546981	H
0.530389	0.681894	0.257171	H
0.357977	0.765805	0.342262	H
0.446725	0.968597	0.978559	H
0.358786	0.028417	0.227742	H
0.396387	0.104459	0.453022	H
0.532986	0.994284	0.203266	H
0.306954	0.585823	0.731859	H
0.33767	0.265995	0.82878	H
0.306423	0.278615	0.127144	H
0.300746	0.407969	0.502348	H
0.302872	0.651982	0.220632	H
0.27713	0.241236	0.337729	H

0.309173	0.85088	0.107266	H
0.335905	0.993638	0.783242	H
0.348454	0.754331	0.792112	H
0.664105	0.006282	0.216768	H
0.690762	0.149164	0.89272	H
0.651553	0.245572	0.207965	H

POSCAR file of the $Au_{32}(Me_3P)_{12}Cl_8$ assembly system

1				
6.531034	7.085206	30.750431		
18.48558	0	0		
8.182881	16.776388	0		
Au	Cl	P	C	H
64	16	24	72	216
direct				
0.993639	0.054173	0.848145	Au	
0.933765	0.125188	0.94799	Au	
0.960483	0.257798	0.947232	Au	
0.97705	0.221327	0.789738	Au	
0.89262	0.165951	0.074143	Au	
0.907717	0.082927	0.841098	Au	
0.858158	0.046275	0.037773	Au	
0.931569	0.959597	0.976963	Au	
0.949352	0.795622	0.004624	Au	
0.958726	0.937367	0.834534	Au	
0.068425	0.04044	0.02297	Au	
0.050617	0.204293	0.995407	Au	
0.04127	0.06262	0.16543	Au	
0.973834	0.850712	0.098515	Au	
0.936391	0.857416	0.247573	Au	
0.881469	0.87918	0.131836	Au	
0.924066	0.000485	0.113078	Au	
0.026146	0.149293	0.901487	Au	
0.063607	0.142573	0.752418	Au	
0.118419	0.121123	0.867805	Au	
0.075884	0.999511	0.886934	Au	
0.018643	0.88686	0.934339	Au	
0.055666	0.970874	0.769824	Au	
0.98123	0.113019	0.065709	Au	
0.944331	0.0291	0.230183	Au	
0.006359	0.945822	0.151845	Au	
0.066219	0.874819	0.051979	Au	

0.039498	0.742194	0.052782	Au
0.02295	0.778677	0.210254	Au
0.107311	0.834121	0.925727	Au
0.09228	0.917078	0.158891	Au
0.141804	0.953773	0.96214	Au
0.573311	0.582587	0.947118	Au
0.426712	0.417425	0.052938	Au
0.489248	0.662347	0.949242	Au
0.510852	0.337772	0.050771	Au
0.425169	0.555213	0.083564	Au
0.574866	0.444837	0.916374	Au
0.474749	0.408399	0.168057	Au
0.525266	0.591779	0.831989	Au
0.5632	0.425305	0.07781	Au
0.436935	0.574883	0.921938	Au
0.511132	0.558342	0.09875	Au
0.488889	0.441691	0.901299	Au
0.642052	0.46403	0.964481	Au
0.358004	0.53598	0.035493	Au
0.613795	0.585098	0.795854	Au
0.386133	0.415402	0.204068	Au
0.55965	0.723492	0.815235	Au
0.440938	0.276838	0.18501	Au
0.463419	0.726601	0.807501	Au
0.537171	0.274264	0.192445	Au
0.401563	0.703117	0.96205	Au
0.598614	0.296975	0.037863	Au
0.449304	0.684638	0.092725	Au
0.550681	0.31537	0.907337	Au
0.547425	0.704851	0.001386	Au
0.45263	0.295189	0.99866	Au
0.438401	0.526706	0.229713	Au
0.561593	0.473319	0.770297	Au
0.598246	0.538178	0.094144	Au
0.401796	0.461904	0.905865	Au
0.538789	0.430307	0.22915	Au
0.461226	0.56968	0.770855	Au
0.785072	0.075685	0.029289	Cl
0.950159	0.332413	0.686361	Cl
0.916714	0.688832	0.011358	Cl
0.083235	0.311171	0.988601	Cl
0.082814	0.950108	0.648774	Cl
0.917046	0.048829	0.351738	Cl

0.214939	0.924219	0.970333	Cl
0.049846	0.667575	0.31361	Cl
0.416065	0.523503	0.362049	Cl
0.583864	0.476446	0.637976	Cl
0.717826	0.455075	0.949511	Cl
0.28224	0.544669	0.050685	Cl
0.576671	0.810424	0.00368	Cl
0.423342	0.189687	0.99633	Cl
0.449228	0.837219	0.68999	Cl
0.550897	0.162944	0.309913	Cl
0.834426	0.200168	0.159164	P
0.972083	0.38968	0.872027	P
0.853391	0.166704	0.782175	P
0.958761	0.864021	0.764548	P
0.041193	0.135969	0.235427	P
0.909056	0.794812	0.382907	P
0.090888	0.204952	0.617034	P
0.165556	0.799859	0.840767	P
0.027904	0.610301	0.127963	P
0.146607	0.833266	0.217794	P
0.829513	0.799679	0.157518	P
0.170418	0.200406	0.842322	P
0.528696	0.363858	0.367712	P
0.471314	0.636129	0.63233	P
0.657198	0.588323	0.092284	P
0.342885	0.411591	0.907767	P
0.678168	0.568673	0.712928	P
0.321763	0.431407	0.287092	P
0.559856	0.859702	0.761219	P
0.440373	0.14071	0.239055	P
0.341994	0.791643	0.945256	P
0.658081	0.208289	0.054742	P
0.437808	0.773663	0.150198	P
0.562163	0.226382	0.849825	P
0.798099	0.120487	0.217816	C
0.846246	0.223992	0.235288	C
0.800343	0.287417	0.106018	C
0.978847	0.442268	0.929687	C
0.930548	0.450461	0.816733	C
0.021781	0.402603	0.793093	C
0.807587	0.115252	0.79552	C
0.829538	0.242115	0.823	C
0.870294	0.224253	0.672892	C

0.000318	0.779847	0.781604	C
0.969638	0.919341	0.654436	C
0.908633	0.817925	0.793052	C
0.999593	0.220076	0.218296	C
0.030294	0.08065	0.345546	C
0.091294	0.182157	0.206938	C
0.868584	0.854172	0.429895	C
0.883868	0.703144	0.413066	C
0.951471	0.761626	0.439591	C
0.131345	0.145486	0.570161	C
0.116017	0.296738	0.586717	C
0.048414	0.237743	0.560526	C
0.201892	0.879539	0.78205	C
0.153756	0.775917	0.764705	C
0.199648	0.712637	0.893961	C
0.021153	0.55775	0.070246	C
0.06944	0.549507	0.183256	C
0.978184	0.597339	0.206864	C
0.192425	0.884714	0.204392	C
0.17045	0.757869	0.17695	C
0.129747	0.775665	0.327078	C
0.8415	0.69103	0.205408	C
0.778409	0.821968	0.220345	C
0.815315	0.816296	0.064037	C
0.158496	0.309071	0.794482	C
0.221523	0.178069	0.779541	C
0.184555	0.183649	0.935906	C
0.521284	0.427847	0.422139	C
0.478564	0.572051	0.578055	C
0.571985	0.287119	0.402477	C
0.428105	0.713083	0.597562	C
0.48035	0.309723	0.41244	C
0.519772	0.689942	0.587674	C
0.697912	0.51128	0.138011	C
0.302157	0.488595	0.862046	C
0.68687	0.646652	0.990243	C
0.313256	0.353149	0.009797	C
0.645095	0.656275	0.143552	C
0.355014	0.34368	0.856447	C
0.674768	0.59506	0.608893	C
0.325097	0.404877	0.391193	C
0.703126	0.465701	0.746867	C
0.296821	0.534385	0.25319	C

0.720349	0.626526	0.703121	C
0.279614	0.373619	0.296662	C
0.604431	0.896078	0.773739	C
0.39575	0.104854	0.226123	C
0.560515	0.909105	0.652868	C
0.439475	0.091168	0.347483	C
0.511607	0.907325	0.80763	C
0.488588	0.092915	0.192764	C
0.303641	0.762045	0.910887	C
0.696449	0.237805	0.089148	C
0.353471	0.892171	0.868037	C
0.646543	0.107787	0.131946	C
0.310057	0.806233	0.035911	C
0.689986	0.193722	0.964066	C
0.429057	0.879998	0.085236	C
0.570843	0.120037	0.914811	C
0.392006	0.753797	0.237713	C
0.607973	0.246185	0.762333	C
0.483727	0.768289	0.190492	C
0.516236	0.231861	0.809491	C
0.76903	0.140006	0.255814	H
0.788479	0.103819	0.175229	H
0.865103	0.171588	0.273627	H
0.866088	0.275831	0.204343	H
0.789517	0.276315	0.06118	H
0.771608	0.300253	0.149309	H
0.006892	0.411153	0.957831	H
0.984863	0.505804	0.889325	H
0.928638	0.424428	0.774723	H
0.898859	0.44881	0.859802	H
0.0491	0.370362	0.822803	H
0.019257	0.375602	0.752437	H
0.793653	0.085132	0.861654	H
0.782572	0.158682	0.765049	H
0.803661	0.281543	0.792184	H
0.815911	0.210888	0.889123	H
0.895939	0.261804	0.662237	H
0.88372	0.182955	0.642009	H
0.032218	0.804163	0.760918	H
0.994541	0.741394	0.847686	H
0.001948	0.942242	0.634432	H
0.969564	0.879758	0.624201	H
0.903094	0.777672	0.85885	H

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0.967714	0.195691	0.238917	H
0.005383	0.258481	0.152203	H
0.998006	0.057672	0.365533	H
0.030319	0.120274	0.375766	H
0.096829	0.222388	0.141133	H
0.118659	0.135124	0.217471	H
0.8398	0.870838	0.403436	H
0.88217	0.910438	0.415972	H
0.907792	0.661022	0.391733	H
0.856133	0.718165	0.384132	H
0.977425	0.723898	0.415083	H
0.938252	0.727343	0.505343	H
0.16013	0.128842	0.596612	H
0.117731	0.089219	0.584186	H
0.092082	0.338836	0.608062	H
0.143752	0.281767	0.615645	H
0.022449	0.275494	0.584988	H
0.061571	0.271972	0.494733	H
0.230947	0.859977	0.744054	H
0.211535	0.896216	0.824604	H
0.134868	0.828259	0.726377	H
0.133941	0.724036	0.795702	H
0.210485	0.723755	0.938774	H
0.228376	0.699797	0.850657	H
0.993109	0.588883	0.0421	H
0.015137	0.494207	0.110568	H
0.071343	0.575527	0.225281	H
0.101132	0.551179	0.140185	H
0.95088	0.629577	0.177112	H
0.980673	0.624303	0.247576	H
0.206336	0.914823	0.138252	H
0.217451	0.841296	0.23484	H
0.196342	0.718456	0.20773	H
0.184058	0.789091	0.110819	H
0.104109	0.738093	0.337754	H
0.116331	0.816927	0.358005	H
0.8686	0.673429	0.162564	H
0.851335	0.673962	0.262956	H
0.768056	0.886736	0.190557	H
0.753159	0.785568	0.227235	H
0.843858	0.795456	0.026097	H
0.78751	0.782399	0.077668	H

0.131392	0.326671	0.83732	H
0.148695	0.326208	0.736891	H
0.23186	0.113291	0.809316	H
0.246784	0.214423	0.772701	H
0.155996	0.204497	0.973812	H
0.212369	0.217469	0.9224	H
0.026953	0.467235	0.757657	H
0.938827	0.513567	0.781374	H
0.949527	0.44041	0.978254	H
0.842549	0.263322	0.648072	H
0.855274	0.278616	0.813604	H
0.818705	0.069358	0.769904	H
0.217068	0.190556	0.718755	H
0.192787	0.118483	0.968772	H
0.187086	0.340435	0.782317	H
0.973015	0.5327	0.242249	H
0.050472	0.55964	0.021672	H
0.061169	0.486396	0.218594	H
0.815884	0.238945	0.274075	H
0.815857	0.067252	0.257087	H
0.819277	0.340473	0.072596	H
0.859019	0.819865	0.496701	H
0.872516	0.674001	0.480133	H
0.965539	0.815309	0.430721	H
0.812928	0.659579	0.21767	H
0.782884	0.809521	0.281107	H
0.80704	0.88144	0.031164	H
0.157514	0.736613	0.35183	H
0.181321	0.930626	0.229987	H
0.144717	0.721347	0.186383	H
0.12737	0.325867	0.519651	H
0.034397	0.183933	0.569597	H
0.140908	0.17971	0.503342	H
0.184126	0.760987	0.725917	H
0.180723	0.659568	0.927396	H
0.184134	0.932762	0.742772	H
0.944942	0.970777	0.637617	H
0.999505	0.744379	0.747517	H
0.91088	0.782544	0.757193	H
0.000325	0.25561	0.252363	H
0.055018	0.02927	0.362377	H
0.089005	0.217572	0.242782	H
0.492334	0.470695	0.408951	H

0.507465	0.529073	0.591284	H
0.516405	0.391157	0.488602	H
0.483465	0.608645	0.51157	H
0.574705	0.24208	0.376985	H
0.425522	0.758095	0.623026	H
0.602958	0.314607	0.380489	H
0.397076	0.68578	0.619588	H
0.452056	0.35379	0.397873	H
0.54799	0.645655	0.60227	H
0.483608	0.266127	0.385149	H
0.516646	0.733445	0.615016	H
0.709161	0.473457	0.102738	H
0.290879	0.52643	0.897296	H
0.725719	0.539039	0.135994	H
0.274376	0.460806	0.864005	H
0.715017	0.670094	0.992964	H
0.28512	0.329691	0.007058	H
0.698113	0.60686	0.957087	H
0.301991	0.392887	0.043009	H
0.62334	0.708066	0.11224	H
0.376775	0.291898	0.887755	H
0.628331	0.625215	0.207819	H
0.37179	0.374779	0.792195	H
0.651017	0.558445	0.610554	H
0.34884	0.441454	0.389621	H
0.662909	0.659245	0.581351	H
0.336962	0.340688	0.418678	H
0.733757	0.460512	0.703133	H
0.266173	0.539597	0.296874	H
0.709622	0.448411	0.807548	H
0.290362	0.5517	0.192473	H
0.726804	0.607003	0.764109	H
0.273222	0.393247	0.235606	H
0.750502	0.616267	0.660924	H
0.249435	0.383858	0.338811	H
0.602563	0.873896	0.839948	H
0.397703	0.12712	0.159873	H
0.635669	0.872193	0.745176	H
0.364542	0.128943	0.254561	H
0.560183	0.975202	0.630526	H
0.439702	0.025104	0.369783	H
0.531313	0.894666	0.643725	H
0.468648	0.105414	0.356897	H

0.48295	0.892108	0.797658	H
0.517255	0.107937	0.202887	H
0.509828	0.882719	0.873835	H
0.490424	0.117599	0.126533	H
0.294117	0.701135	0.954871	H
0.705983	0.298708	0.045173	H
0.274827	0.806542	0.905425	H
0.72525	0.193276	0.094583	H
0.373485	0.919076	0.887292	H
0.6265	0.080934	0.112693	H
0.372262	0.887175	0.810573	H
0.627767	0.112797	0.189413	H
0.280823	0.84822	0.022175	H
0.719215	0.151702	0.977751	H
0.300179	0.747181	0.083659	H
0.699864	0.252772	0.916319	H
0.400563	0.89027	0.059523	H
0.599321	0.109658	0.940596	H
0.423913	0.917801	0.11974	H
0.575954	0.082238	0.880314	H
0.361784	0.761378	0.217821	H
0.638196	0.238552	0.78224	H
0.396697	0.690426	0.281428	H
0.603304	0.309565	0.718618	H
0.512863	0.783839	0.139804	H
0.487095	0.216344	0.860168	H
0.477164	0.810111	0.221013	H
0.522776	0.19006	0.778952	H
0.397799	0.038189	0.254174	H
0.41031	0.114326	0.381892	H
0.487514	0.026749	0.219847	H
0.677141	0.069101	0.141311	H
0.680541	0.240165	0.148856	H
0.669942	0.169899	0.941834	H
0.602209	0.962752	0.745655	H
0.589655	0.886096	0.618278	H
0.512589	0.973515	0.780478	H
0.330073	0.830097	0.058152	H
0.322853	0.930788	0.858677	H
0.319553	0.759654	0.851191	H
0.290815	0.308848	0.319415	H
0.319779	0.57434	0.24757	H
0.293081	0.416054	0.428378	H

0.316694	0.526551	0.798232	H
0.335414	0.302584	0.041025	H
0.324905	0.321851	0.85925	H
0.510438	0.294267	0.765287	H
0.54202	0.102642	0.965509	H
0.610589	0.204963	0.732475	H
0.449844	0.538278	0.599188	H
0.435608	0.742876	0.53013	H
0.523926	0.722118	0.52073	H
0.564485	0.25731	0.469906	H
0.549938	0.461774	0.401075	H
0.476256	0.27759	0.479375	H
0.706774	0.58385	0.571694	H
0.680168	0.42572	0.75254	H
0.709138	0.691293	0.68032	H
0.664734	0.697228	0.958961	H
0.675216	0.6781	0.140709	H
0.683395	0.473314	0.201828	H
0.489552	0.7059	0.234706	H
0.457849	0.897484	0.034483	H
0.389366	0.795036	0.267563	H

POSCAR file of the $Au_{32}(P_3H)_{12}Cl_8$ assembly system

1			
7.193192	5.874932	29.470342	
18.435348	0	0	
8.46119	16.532558	0	
Au	Cl	P	H
64	16	24	72
direct			
0.994584	0.057464	0.845555	Au
0.930632	0.128487	0.944796	Au
0.958646	0.259617	0.944672	Au
0.975635	0.226106	0.785664	Au
0.88611	0.167209	0.06982	Au
0.903281	0.092427	0.835366	Au
0.851217	0.050856	0.034735	Au
0.927272	0.963056	0.974162	Au
0.951097	0.796237	0.998257	Au
0.958552	0.946268	0.829015	Au
0.073429	0.037009	0.024622	Au
0.048643	0.203318	0.001863	Au

0.042368	0.053901	0.169101	Au
0.971914	0.846872	0.100083	Au
0.935613	0.845751	0.24972	Au
0.875252	0.881186	0.131045	Au
0.919542	0.997707	0.115359	Au
0.02934	0.152255	0.898853	Au
0.065198	0.152898	0.749275	Au
0.126168	0.117085	0.865533	Au
0.081019	0.00044	0.884419	Au
0.020298	0.888526	0.936126	Au
0.057279	0.965485	0.772535	Au
0.980188	0.110037	0.062628	Au
0.943247	0.033976	0.226203	Au
0.006354	0.941322	0.154077	Au
0.070134	0.870971	0.054326	Au
0.041222	0.739939	0.053623	Au
0.025806	0.773045	0.213005	Au
0.114374	0.831668	0.929788	Au
0.097555	0.907181	0.163682	Au
0.149395	0.948375	0.96469	Au
0.570406	0.581957	0.947266	Au
0.42915	0.418813	0.052678	Au
0.484541	0.66962	0.950584	Au
0.515158	0.33071	0.04935	Au
0.420633	0.558715	0.081297	Au
0.578057	0.442329	0.919189	Au
0.477672	0.40323	0.171757	Au
0.521103	0.598918	0.827163	Au
0.568545	0.418106	0.08123	Au
0.430885	0.583045	0.91842	Au
0.509189	0.55734	0.101507	Au
0.490108	0.443885	0.898704	Au
0.647157	0.472475	0.96164	Au
0.352111	0.527859	0.037815	Au
0.613552	0.586782	0.796397	Au
0.385404	0.41401	0.203159	Au
0.554104	0.729307	0.808377	Au
0.445718	0.271273	0.191394	Au
0.455811	0.740493	0.808167	Au
0.543061	0.261623	0.192464	Au
0.394968	0.717046	0.959198	Au
0.604572	0.283639	0.0406	Au
0.439072	0.685123	0.098767	Au

0.560219	0.31625	0.900192	Au
0.549869	0.700018	0.004806	Au
0.450063	0.300256	0.995133	Au
0.434559	0.526636	0.230198	Au
0.564843	0.475417	0.769633	Au
0.599733	0.538202	0.093798	Au
0.399546	0.46195	0.907218	Au
0.545076	0.425707	0.230941	Au
0.453966	0.573678	0.76906	Au
0.787625	0.115157	0.977086	Cl
0.928091	0.331644	0.708191	Cl
0.905489	0.716097	0.992461	Cl
0.089748	0.291169	0.006551	Cl
0.097835	0.952705	0.652266	Cl
0.904805	0.047373	0.346811	Cl
0.213221	0.885421	0.021959	Cl
0.072124	0.664755	0.290592	Cl
0.411256	0.486688	0.370594	Cl
0.588467	0.513929	0.629438	Cl
0.724315	0.440664	0.96446	Cl
0.274947	0.56001	0.034792	Cl
0.566187	0.82117	0.996294	Cl
0.434272	0.178885	0.003218	Cl
0.443264	0.827795	0.678028	Cl
0.556427	0.173805	0.321958	Cl
0.838292	0.201081	0.169837	P
0.949787	0.396901	0.872033	P
0.848408	0.191946	0.774951	P
0.945467	0.876748	0.765951	P
0.050742	0.120305	0.239218	P
0.89878	0.828988	0.378556	P
0.102401	0.171146	0.620149	P
0.161777	0.797505	0.829668	P
0.053507	0.603984	0.131284	P
0.15263	0.807987	0.223944	P
0.838548	0.77639	0.156027	P
0.163094	0.221273	0.841824	P
0.529605	0.359307	0.371696	P
0.469996	0.641577	0.62839	P
0.664719	0.569733	0.0982	P
0.334383	0.431492	0.902129	P
0.675256	0.580619	0.699772	P
0.323833	0.41935	0.300227	P

0.569925	0.856956	0.771133	P
0.430082	0.1436	0.228138	P
0.31991	0.764658	0.974472	P
0.679612	0.235811	0.025582	P
0.443141	0.800634	0.109526	P
0.556826	0.200449	0.88947	P
0.919733	0.771081	0.445531	H
0.854835	0.803338	0.409574	H
0.891079	0.900935	0.393385	H
0.19427	0.832357	0.217864	H
0.16881	0.74601	0.19472	H
0.142156	0.758887	0.310081	H
0.057474	0.547753	0.096345	H
0.020339	0.569679	0.203185	H
0.092741	0.5736	0.167009	H
0.207781	0.811844	0.80822	H
0.14948	0.838973	0.750557	H
0.169033	0.714657	0.839979	H
0.209411	0.202651	0.848983	H
0.144263	0.261291	0.896025	H
0.167075	0.290023	0.763902	H
0.082031	0.230607	0.553007	H
0.10989	0.100092	0.603908	H
0.14658	0.195738	0.590634	H
0.982725	0.826447	0.740292	H
0.928777	0.920189	0.691307	H
0.914129	0.818536	0.813097	H
0.858619	0.240427	0.688674	H
0.832695	0.254215	0.803809	H
0.806581	0.167444	0.782185	H
0.907428	0.436053	0.848423	H
0.978799	0.429388	0.79384	H
0.955959	0.448187	0.905946	H
0.799178	0.159841	0.211653	H
0.816966	0.283143	0.149769	H
0.85611	0.185739	0.239082	H
0.825876	0.778152	0.087414	H
0.796697	0.763709	0.213682	H
0.86123	0.695164	0.18605	H
0.036857	0.206223	0.207296	H
0.094806	0.119598	0.249174	H
0.027404	0.096696	0.322433	H
0.513686	0.615472	0.590849	H

0.470816	0.727239	0.59921	H
0.442675	0.641959	0.577902	H
0.294231	0.461159	0.945555	H
0.328396	0.347473	0.934445	H
0.321821	0.459438	0.824765	H
0.303838	0.824505	0.902626	H
0.299989	0.804774	0.027547	H
0.290315	0.704008	0.003119	H
0.414027	0.873608	0.073214	H
0.486481	0.829833	0.074614	H
0.435135	0.798064	0.189676	H
0.292864	0.36058	0.333074	H
0.292142	0.49169	0.280063	H
0.331864	0.414019	0.374319	H
0.528786	0.273489	0.402252	H
0.486123	0.385805	0.409519	H
0.557384	0.360081	0.420832	H
0.699578	0.19552	0.972666	H
0.695661	0.176148	0.097516	H
0.70919	0.29653	0.996767	H
0.513731	0.170355	0.924843	H
0.586391	0.12812	0.925562	H
0.564832	0.202811	0.809399	H
0.70671	0.507962	0.720063	H
0.706471	0.638961	0.667011	H
0.667174	0.586121	0.625641	H
0.615943	0.871183	0.749947	H
0.553575	0.889517	0.831231	H
0.5543	0.922744	0.7015	H
0.670156	0.654019	0.065801	H
0.704949	0.54079	0.054347	H
0.677515	0.542157	0.175299	H
0.446431	0.111756	0.167465	H
0.384108	0.129128	0.249345	H
0.44588	0.077511	0.297406	H

POSCAR file of the $Au_{32}H_{12}Cl_8$ assembly system

1		
-0.427731	-7.298516	-25.131436
8.482607	-14.660973	0
-8.013962	-14.660973	0
Au	Cl	H

	64	16	24
Direct			
	-0.018457	0.123393	-0.911408
	-0.046048	0.962378	-1.878727
	-0.011542	0.789782	-1.741188
	-0.019094	0.876115	-1.632132
	-0.123357	0.847908	-1.809461
	-0.128485	0.173828	-0.882746
	-0.144155	0.039154	-0.930749
	-0.050851	0.12312	-1.065449
	-0.043481	0.371231	-1.221426
	-0.068667	0.288806	-1.036291
	-0.949374	0.871791	-0.933007
	-0.953651	0.629	-0.778941
	-0.931197	0.710428	-0.963993
	-0.040143	0.046363	-0.192033
	-0.036901	0.912446	-1.241972
	-0.137651	0.106557	-0.121414
	-0.078166	0.940535	-1.008611
	-0.961382	0.951746	-1.806322
	-0.967665	0.087231	-0.757058
	-0.864554	0.888786	-1.873945
	-0.92336	0.055468	-0.990193
	-0.969892	0.225262	-1.116235
	-0.929689	0.201896	-0.933241
	-0.030928	0.771124	-0.882655
	-0.071717	0.790919	-1.066261
	-0.984871	0.871875	-1.08933
	-0.954127	0.029601	-0.118789
	-0.986947	0.204115	-0.256792
	-0.983769	0.121547	-0.367265
	-0.877902	0.146677	-0.19007
	-0.874651	0.830217	-1.120063
	-0.855303	0.957065	-1.065098
	-0.393168	0.880563	-1.433447
	-0.606882	0.130104	-0.60883
	-0.495582	0.9059	-1.33638
	-0.498524	0.130394	-0.678619
	-0.538866	0.964825	-1.503665
	-0.457797	0.055665	-0.50943
	-0.520833	0.857998	-1.586481
	-0.494318	0.129747	-0.381465
	-0.432046	0.941361	-1.594883

-0.575804	0.081385	-0.427471
-0.475538	0.790072	-1.417868
-0.52172	0.229912	-0.580739
-0.320602	0.969543	-1.607926
-0.678942	0.046861	-0.421583
-0.396764	0.037924	-0.388156
-0.631487	0.961208	-1.557415
-0.377686	0.856732	-1.265777
-0.562252	0.038878	-0.713418
-0.557916	0.992123	-1.244565
-0.459942	0.025978	-0.779722
-0.605912	0.907367	-1.311416
-0.391868	0.106227	-0.704253
-0.548624	0.738195	-1.23105
-0.428021	0.277942	-0.73015
-0.429637	0.733664	-1.260445
-0.572082	0.295897	-0.731518
-0.587615	0.806431	-1.417855
-0.420227	0.209151	-0.534463
-0.339167	0.773142	-1.528746
-0.630679	0.254292	-0.548963
-0.42409	0.76242	-1.579434
-0.581357	0.255327	-0.424303
-0.201754	0.093115	-0.825388
-0.007645	0.990484	-1.601949
-0.009197	0.382065	-1.366258
-0.986842	0.612826	-0.631906
-0.908783	0.300976	-1.093838
-0.089604	0.69156	-0.905066
-0.79741	0.898212	-1.165713
-0.000265	0.011633	-0.399035
-0.632057	0.680349	-1.326162
-0.419775	0.367716	-0.665233
-0.276095	0.82898	-1.498859
-0.719062	0.198743	-0.513593
-0.483306	0.607205	-1.184885
-0.56502	0.428209	-0.870621
-0.571652	0.99104	-1.105845
-0.371127	0.988782	-1.814443
-0.163885	0.78352	-1.723089
-0.032775	0.7832	-1.627218
-0.09036	0.255297	-0.911695
-0.075956	0.401187	-1.137774

-0.919586	0.600268	-0.863397
-0.071347	0.816702	-1.180649
-0.930317	0.178897	-0.819491
-0.838741	0.212719	-0.277879
-0.96593	0.210669	-0.370642
-0.921498	0.763568	-1.096153
-0.167973	0.183302	-0.206631
-0.83524	0.812328	-1.787235
-0.481452	0.784956	-1.62893
-0.535884	0.210645	-0.346512
-0.360987	0.701734	-1.552589
-0.634656	0.314289	-0.485824
-0.356392	0.961372	-1.2996
-0.677479	0.018577	-0.620406
-0.38217	0.73794	-1.204008
-0.52094	0.070064	-0.82118
-0.671056	0.933151	-1.339996
-0.322887	0.081518	-0.702528
-0.609506	0.795271	-1.211313
-0.419465	0.223336	-0.793165

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