A "gold standard" computational proof for the existence of gold(III) aurophilicity

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Electronic Supplementary Information (ESI)

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1. Computational details.

The calculations were carried out using TURBOMOLE version 7.5.1.[1] The optimized structures were visualized and rendered using UCSF ChimeraX.[2] The QTAIM descriptors and IRI isosurfaces were computed with Multiwfn,[3] and visualized and rendered with VMD.[4]

The structure of $[Au^{III}(CH_3)_3(NH_3)]_2$ (molecule **1**) was built from scratch and optimized at the RI-MP2 level of theory[5–7] with def2-TZVP basis sets[7–9] for all atoms and a 60-electron effective core potential for gold (def2-ECP).[10] The structure of $[Au^{III}(N_3)_4]_2^{2-}$ (molecule **2**) was extracted from the X-ray structure of $[NMe_4][Au^{III}(N_3)_4]$[11] and optimized using the same procedure. The structure of $\{cis\text{-}[Au^{III}(CH_3)_2(NH_3)_2]\}_2^{2+}$ (molecule **3**) was built from the optimized structure of molecule **1** keeping the $Au^{III}\cdots Au^{III}$ distance frozen and optimized using the same procedure. The three structures were constrained to the C_2 point group for reducing the computational efforts. The internal coordinate corresponding to the gold(III)···gold(III) distance was manually stretched to the selected values while all other internal coordinates were kept intact. The interaction energies between $[Au^{III}(CH_3)_3(NH_3)]_2$, $[Au^{III}(N_3)_4]_2^{2-}$ and $\{cis\text{-}[Au^{III}(CH_3)_2(NH_3)_2]\}_2^{2+}$ monomers, respectively, were calculated at the RHF,[12] RI-MP2,[5–7] and CCSD(T)[13] levels of theory using Eq. S1 for the counterpoise correction of the basis set superposition error,[14,15]

$$\Delta E_{\text{int}} = E_{\text{AB}}^{(\text{AB})} - E_{\text{A}}^{(\text{AB})} - E_{\text{B}}^{(\text{AB})} \quad \text{(S1)}$$

where ΔE_{int} is the interaction energy, and $E_{\text{AB}}^{(\text{AB})}$, $E_{\text{A}}^{(\text{AB})}$, $E_{\text{B}}^{(\text{AB})}$ are the energies of the dimer and monomers, respectively, calculated using the basis sets of the dimer. The calculation points were fitted using Eq. S2, which has been previously used to derive the Herschbach-Laurie relation,[16]

$$\Delta E_{\text{int}}\,(R) = A \cdot \exp(-B \cdot R) - C \cdot R^{D} \quad \text{(S2)}$$

where R is the gold(III)···gold(III) distance and A, B, C, D are fitting parameters.

The contribution from the $Au^{III}\cdots$[ligand] and interligand interactions to the total interaction energy of molecule **1** has been partially removed by subtracting twice that calculated for a monomer of **1** and the saturated ligands of the other monomer at the RI-MP2 and CCSD(T) $Au^{III}\cdots Au^{III}$ equilibrium distances, respectively. The extra [ligand]···[ligand] interaction energy that has been removed this way has been restored by adding that of the saturated ligands of $[(CH_4)_3(NH_3)]_2$ Then, the gold(III) atoms were manually removed from molecule **1** at the RI-MP2 and CCSD(T) $Au^{III}\cdots Au^{III}$ equilibrium distances and replaced with hydrogen atoms attached to the carbon atoms. The position of the added hydrogen atoms was refined by optimizing the structure at the RI-MP2/def2-TZVP level of theory while keeping all other positions of the atoms fixed. Interaction energy calculations were then carried out.

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2. Interaction energy calculations on molecules *1-3*.

Table S1. Absolute energies of the dimer ($E_{AB}^{(AB)}$ in Hartree) and monomers ($E_{A}^{(AB)}$ in Hartree), calculated using the basis sets of the dimer, and interaction energies (ΔE_{int} in Hartree and kJ·mol^{-1}) as a function of the Au^{III}···Au^{III} distance (R in Å) for molecule **1** at the RHF, RI-MP2 and CCSD(T) levels of theory

	RHF				RI-MP2				CCSD(T)			
R	$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}		$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}		$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}	
			Ha	kJ·mol^{-1}			Ha	kJ·mol^{-1}			Ha	kJ·mol^{-1}
2.80	-619.56997	-309.81949	0.06902	181.20495	-622.15261	-311.08378	0.01495	39.25646	-622.24321	-311.13568	0.02815	73.91991
3.00	-619.60580	-309.81943	0.03306	86.79141	-622.17289	-311.08244	-0.00800	-21.00395	-622.26687	-311.13427	0.00167	4.37502
3.20	-619.62551	-309.81937	0.01323	34.73135	-622.18086	-311.08139	-0.01808	-47.47626	-622.27723	-311.13314	-0.01095	-28.73994
3.40	-619.63599	-309.81933	0.00266	6.98846	-622.18239	-311.08052	-0.02135	-56.06746	-622.28043	-311.13220	-0.01602	-42.06491
3.48	-619,63856	-309,81931	6,16027E-5	0,16174	-622,18201	-311,08022	-0,02158	-56,64586	-	-	-	-
3.60	-619.64125	-309.81929	-0.00267	-6.99847	-622.18081	-311.07980	-0.02120	-55.67190	-622.28000	-311.13142	-0.01716	-45.05078
3.80	-619.64362	-309.81926	-0.00509	-13.35716	-622.17793	-311.07922	-0.01949	-51.18338	-622.27795	-311.13078	-0.01638	-43.00517
4.00	-619.64442	-309.81924	-0.00594	-15.59703	-622.17475	-311.07877	-0.01722	-45.19857	-622.27537	-311.13029	-0.01478	-38.80862
4.20	-619.64441	-309.81921	-0.00598	-15.70392	-622.17170	-311.07842	-0.01487	-39.02831	-622.27279	-311.12992	-0.01294	-33.96481
4.40	-619.64402	-309.81919	-0.00563	-14.78484	-622.16898	-311.07815	-0.01268	-33.28744	-622.27040	-311.12964	-0.01113	-29.22327

[a] $E_{A}^{(AB)}$ is equal to $E_{B}^{(AB)}$ due to the C_2 symmetry

Table S2. Absolute energies of the dimer ($E_{AB}^{(AB)}$ in Hartree) and monomers ($E_{A}^{(AB)}$ in Hartree), calculated using the basis sets of the dimer, and interaction energies (ΔE_{int} in Hartree and kJ·mol^{-1}) as a function of the Au^{III}···Au^{III} distance (R in Å) for molecule **2** at the RHF and RI-MP2 levels of theory

	RHF				RI-MP2			
R	$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}		$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}	
			Ha	kJ·mol^{-1}			Ha	kJ·mol^{-1}
2.80	-1576.07221	-788.11115	0.15008	394.04641	-1582.13373	-791.10468	0.07563	198.55535
3.00	-1576.10115	-788.11098	0.12081	317.19452	-1582.14128	-791.10302	0.06476	170.02780
3.20	-1576.11722	-788.11083	0.10444	274.19763	-1582.14134	-791.10167	0.06201	162.79780
3.40	-1576.12642	-788.11069	0.09496	249.30873	-1582.13846	-791.10055	0.06265	164.48019
3.60	-1576.13196	-788.11056	0.08917	234.10756	-1582.13482	-791.09962	0.06443	169.15321
3.80	-1576.13556	-788.11045	0.08535	224.07625	-1582.13144	-791.09887	0.06630	174.07660
4.00	-1576.13813	-788.11035	0.08258	216.80266	-1582.12869	-791.09826	0.06784	178.11481
4.20	-1576.14015	-788.11026	0.08037	211.00690	-1582.12666	-791.09778	0.06891	180.91810
4.40	-1576.14189	-788.11018	0.07847	206.01451	-1582.12529	-791.09740	0.06951	182.49896

[a] $E_{A}^{(AB)}$ is equal to $E_{B}^{(AB)}$ due to the C_2 symmetry

Table S3. Absolute energies of the dimer ($E_{AB}^{(AB)}$ in Hartree) and monomers ($E_{A}^{(AB)}$ in Hartree), calculated using the basis sets of the dimer, and interaction energies (ΔE_{int} in Hartree and kJ·mol^{-1}) as a function of the Au^{III}···Au^{III} distance (R in Å) for molecule **3** at the RHF and RI-MP2 levels of theory

	RHF				RI-MP2			
R	$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}		$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}	
			Ha	kJ·mol^{-1}			Ha	kJ·mol^{-1}
2.80	-652,37919	-326,26611	0,15304	401,80349	-654,98155	-327,54693	0,11231	294,86866
3.00	-652,40859	-326,26604	0,12349	324,22802	-654,99833	-327,54575	0,09317	244,60800
3.20	-652,42541	-326,26598	0,10655	279,74337	-655,00589	-327,54484	0,08378	219,97353
3.40	-652,43549	-326,26593	0,09638	253,04309	-655,00908	-327,54411	0,07914	207,77573
3.60	-652,44188	-326,26589	0,08991	236,04967	-655,01030	-327,54352	0,07674	201,47313
3.80	-652,44623	-326,26586	0,08549	224,45177	-655,01075	-327,54305	0,07534	197,81423
4.00	-652,44943	-326,26583	0,08224	215,91558	-655,01100	-327,54268	0,07435	195,21499
4.20	-652,45195	-326,26581	0,07966	209,15084	-655,01128	-327,54238	0,07348	192,91565
4.40	-652,45409	-326,26579	0,07748	203,43260	-655,01166	-327,54212	0,07259	190,58782

[a] $E_{A}^{(AB)}$ is equal to $E_{B}^{(AB)}$ due to the C_2 symmetry

Table S4. Absolute energies of the dimer ($E_{AB}^{(AB)}$ in Hartree) and monomers ($E_{A}^{(AB)}$, $E_{B}^{(AB)}$ in Hartree), calculated using the basis sets of the dimer, and interaction energies (ΔE_{int} in Hartree and kJ·mol^{-1}) as a function of the Au^{III}···Au^{III} distance (R in Å) for [Au^{III}(CH$_3$)$_3$(NH$_3$)]···[(CH$_4$)$_3$(NH$_3$)] at the RI-MP2 and CCSD(T) levels of theory

	RI-MP2					CCSD(T)				
R	$E_{AB}^{(AB)}$	$E_{A}^{(AB)}$	$E_{B}^{(AB)}$	ΔE_{int}		$E_{AB}^{(AB)}$	$E_{A}^{(AB)}$	$E_{B}^{(AB)}$	ΔE_{int}	
				Ha	kJ·mol^{-1}				Ha	kJ·mol^{-1}
3.48	-488.69537	-311.07960	-177.60615	-0.00962	-25.25260	-	-	-	-	-
3.59	-	-	-	-	-	-488.84876	-311.13088	-177.70911	-0.00878	-23.05709

Table S5. Absolute energies of the dimer ($E_{AB}^{(AB)}$ in Hartree) and monomers ($E_{A}^{(AB)}$ in Hartree), calculated using the basis sets of the dimer, and interaction energies (ΔE_{int} in Hartree and kJ·mol^{-1}) as a function of the Au^{III}···Au^{III} distance (R in Å) for [(CH$_4$)$_3$(NH$_3$)]$_2$ at the RI-MP2 and CCSD(T) levels of theory

	RI-MP2				CCSD(T)			
R	$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}		$E_{AB}^{(AB)}$	$E_{A}^{(AB)a}$	ΔE_{int}	
			Ha	kJ·mol^{-1}			Ha	kJ·mol^{-1}
3.48	-355.21557	-177.60575	-0.00408	-10.70597	-	-	-	-
3.59	-	-	-	-	-355.42174	-177.70867	-0.00440	-11.55064

[a] $E_{A}^{(AB)}$ is equal to $E_{B}^{(AB)}$ due to the C_2 symmetry

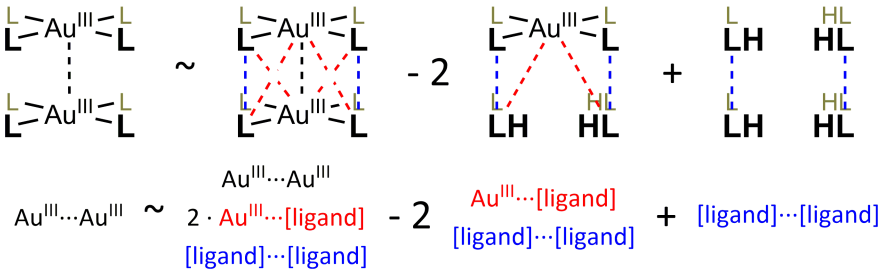

Figure S1. The $Au^{III}\cdots Au^{III}$ interaction energy as the difference between the total interaction energies of molecule **1**, $[Au^{III}(CH_3)_3(NH_3)]\cdots[(CH_4)_3(NH_3)]$, and $[(CH_4)_3(NH_3)]_2$.

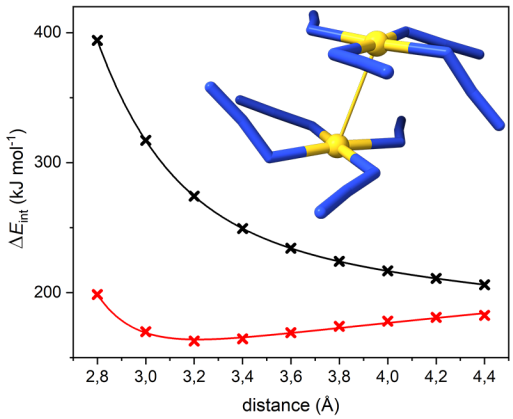

Figure S2. The total interaction energy as a function of the $Au^{III}\cdots Au^{III}$ distance for molecule **2**, calculated at the RHF (black) and RI-MP2 (red) levels of theory. Inset: RI-MP2/def2-TZVP optimized structure of molecule **2**; colour code: Au, yellow; N, blue.

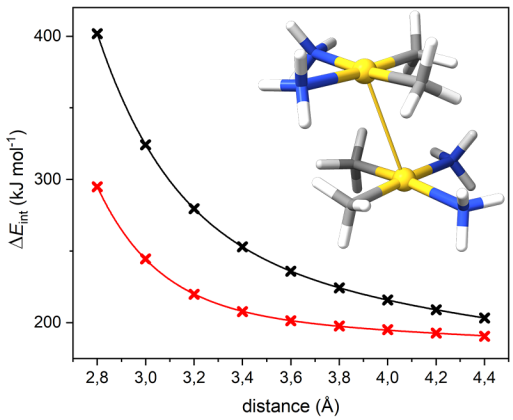

Figure S3. The total interaction energy as a function of the $Au^{III}\cdots Au^{III}$ distance for molecule **3**, calculated at the RHF (black) and RI-MP2 (red) levels of theory. Inset: RI-MP2/def2-TZVP optimized structure of molecule **3**; colour code: C, grey; H, white; Au, yellow; N, blue.

3. Energy decomposition analysis (EDA) of molecule *1*.

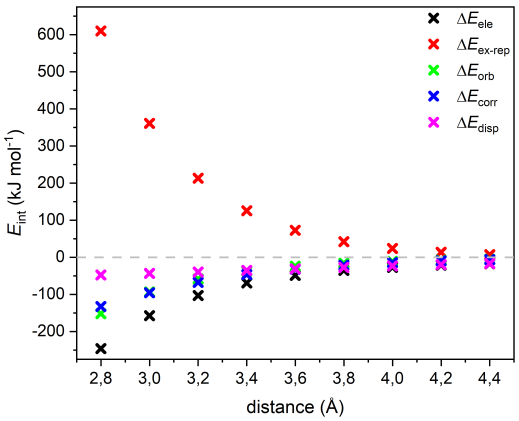

Figure S4. EDA contributions to the total interaction energy between the monomers of molecule **1** as a function of the $Au^{III}\cdots Au^{III}$ distance.

4. Interaction region indicator (IRI) analysis of molecule *2*.

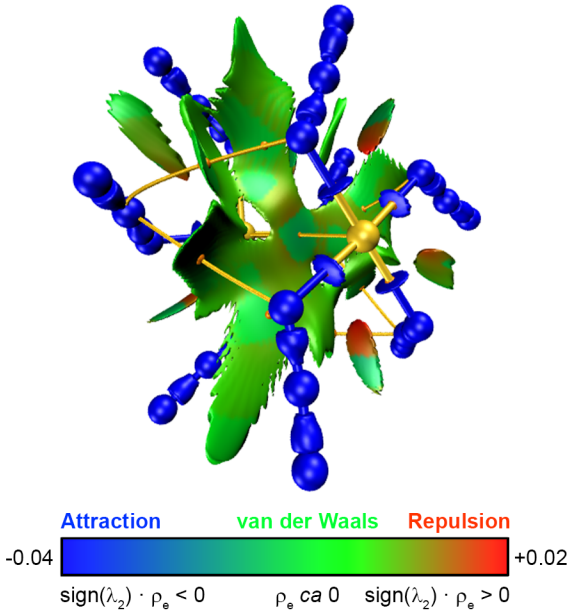

Figure S5. The QTAIM (3, -1) BCPs (orange dots), bond paths (yellow strings) and the IRI isosurface (isovalue = 1.0) are superimposed for molecule **2**. The RGB colour scale refers to the IRI isosurface (adapted from *Chemistry–Methods*, 2021, **1**, 231–239). Colour code: Au, yellow, N, blue.

5. Cartesian coordinates of molecule *1*.

Au	-0.2840909	-1.6626114	0.0038834
Au	0.2840909	1.6626114	0.0038834
C	-1.1406741	-1.6882529	-1.9091007
C	-2.0803616	-1.9079908	0.8766101
C	0.5474621	-1.7428369	1.9029510
C	-0.5474621	1.7428369	1.9029510
C	2.0803616	1.9079908	0.8766101
C	1.1406741	1.6882529	-1.9091007
N	-1.6535393	1.3971633	-0.8760964
N	1.6535393	-1.3971633	-0.8760964
H	-0.7108989	2.7885766	2.1839981
H	-0.1085551	-1.2886236	2.6474035
H	-1.5084909	1.2197318	1.9385997
H	0.7108989	-2.7885766	2.1839981
H	0.1085551	1.2886236	2.6474035
H	1.5084909	-1.2197318	1.9385997
H	-2.3981632	1.7143221	-0.2610313
H	1.7481261	-1.8665163	-1.7729021
H	-1.7481261	1.8665163	-1.7729021
H	2.3981632	-1.7143221	-0.2610313
H	-0.6282005	-1.0191946	-2.6103023
H	2.2101068	1.4526800	-1.9334602
H	0.6282005	1.0191946	-2.6103023
H	-1.0478583	-2.7074868	-2.3011898
H	-2.2101068	-1.4526800	-1.9334602
H	1.0478583	2.7074868	-2.3011898
H	-2.3736470	-0.9567175	1.3268692
H	2.8259726	2.2231370	0.1473673
H	-2.8259726	-2.2231370	0.1473673
H	1.9960736	2.6525242	1.6683523
H	2.3736470	0.9567175	1.3268692
H	-1.9960736	-2.6525242	1.6683523
H	-1.7706642	0.3941646	-1.0319519
H	1.7706642	-0.3941646	-1.0319519

$R(Au^{III}\cdots Au^{III})$ = 2.8 Å

Au	-0.2356740	-1.3800209	0.0039412
Au	0.2356740	1.3800209	0.0039412
C	-1.0926741	-1.4050209	-1.9090588
C	-2.0316740	-1.6250209	0.8769412
C	0.5953259	-1.4600209	1.9029412
C	-0.5953259	1.4600209	1.9029412
C	2.0316740	1.6250209	0.8769412
C	1.0926741	1.4050209	-1.9090588
N	-1.7023259	1.1140209	-0.8760588
N	1.7023259	-1.1140209	-0.8760588
H	-0.7593259	2.5060209	2.1839412
H	-0.0606740	-1.0060209	2.6469412
H	-1.5563259	0.9370209	1.9389412
H	0.7593259	-2.5060209	2.1839412
H	0.0606740	1.0060209	2.6469412
H	1.5563259	-0.9370209	1.9389412
H	-2.4463260	1.4310209	-0.2610588
H	1.7963259	-1.5840209	-1.7730588
H	-1.7963259	1.5840209	-1.7730588
H	2.4463260	-1.4310209	-0.2610588
H	-0.5796741	-0.7360209	-2.6100588
H	2.1616740	1.1700209	-1.9330588
H	0.5796741	0.7360209	-2.6100588
H	-0.9996741	-2.4240209	-2.3010588
H	-2.1616740	-1.1700209	-1.9330588
H	0.9996741	2.4240209	-2.3010588
H	-2.3256740	-0.6740209	1.3269412
H	2.7776741	1.9400209	0.1469412
H	-2.7776741	-1.9400209	0.1469412
H	1.9476741	2.3700209	1.6679412
H	2.3256740	0.6740209	1.3269412
H	-1.9476741	-2.3700209	1.6679412
H	-1.8193260	0.1110209	-1.0320588
H	1.8193260	-0.1110209	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 3.0 Å

Au	-0.2516326	-1.4787431	0.0039412
Au	0.2516326	1.4787431	0.0039412
C	-1.1086177	-1.5042503	-1.9090588
C	-2.0474873	-1.7248061	0.8769412
C	0.5794146	-1.5582511	1.9029412
C	-0.5794146	1.5582511	1.9029412
C	2.0474873	1.7248061	0.8769412
C	1.1086177	1.5042503	-1.9090588
N	-1.6862096	1.2115959	-0.8760588
N	1.6862096	-1.2115959	-0.8760588
H	-0.7440337	2.6041539	2.1839412
H	-0.0768540	-1.1046395	2.6469412
H	-1.5401048	1.0346824	1.9389412
H	0.7440337	-2.6041539	2.1839412
H	0.0768540	1.1046395	2.6469412
H	1.5401048	-1.0346824	1.9389412
H	-2.4303971	1.5281555	-0.2610588
H	1.7804878	-1.6815402	-1.7730588
H	-1.7804878	1.6815402	-1.7730588
H	2.4303971	-1.5281555	-0.2610588
H	-0.5960138	-0.8349468	-2.6100588
H	2.1777566	1.2698832	-1.9330588
H	0.5960138	0.8349468	-2.6100588
H	-1.0150145	-2.5231951	-2.3010588
H	-2.1777566	-1.2698832	-1.9330588
H	1.0150145	2.5231951	-2.3010588
H	-2.3420502	-0.7739803	1.3269412
H	2.7933007	2.0402477	0.1469412
H	-2.7933007	-2.0402477	0.1469412
H	1.9630463	2.4697563	1.6679412
H	2.3420502	0.7739803	1.3269412
H	-1.9630463	-2.4697563	1.6679412
H	-1.8026158	0.2085268	-1.0320588
H	1.8026158	-0.2085268	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 3.2 Å

Au	-0.2675251	-1.5774759	0.0039412
Au	0.2675251	1.5774759	0.0039412
C	-1.1244958	-1.6034629	-1.9090588
C	-2.0632418	-1.8245443	0.8769412
C	0.5635665	-1.6565188	1.9029412
C	-0.5635665	1.6565188	1.9029412
C	2.0632418	1.8245443	0.8769412
C	1.1244958	1.6034629	-1.9090588
N	-1.6701672	1.3092441	-0.8760588
N	1.6701672	-1.3092441	-0.8760588
H	-0.7287711	2.7023292	2.1839412
H	-0.0929560	-1.2032746	2.6469412
H	-1.5239635	1.1324123	1.9389412
H	0.7287711	-2.7023292	2.1839412
H	0.0929560	1.2032746	2.6469412
H	1.5239635	-1.1324123	1.9389412
H	-2.4145318	1.6253870	-0.2610588
H	1.7647085	-1.7791355	-1.7730588
H	-1.7647085	1.7791355	-1.7730588
H	2.4145318	-1.6253870	-0.2610588
H	-0.6122666	-0.9338726	-2.6100588
H	2.1937657	1.3696943	-1.9330588
H	0.6122666	0.9338726	-2.6100588
H	-1.0303222	-2.6223552	-2.3010588
H	-2.1937657	-1.3696943	-1.9330588
H	1.0303222	2.6223552	-2.3010588
H	-2.3583369	-0.8738835	1.3269412
H	2.8088785	2.1404033	0.1469412
H	-2.8088785	-2.1404033	0.1469412
H	1.9783838	2.5694470	1.6679412
H	2.3583369	0.8738835	1.3269412
H	-1.9783838	-2.5694470	1.6679412
H	-1.7860120	0.3061100	-1.0320588
H	1.7860120	-0.3061100	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 3.4 Å

Au	-0.2833620	-1.6762178	0.0039412
Au	0.2833620	1.6762178	0.0039412
C	-1.1403188	-1.7026565	-1.9090588
C	-2.0789481	-1.9242326	0.8769412
C	0.5477712	-1.7548226	1.9029412
C	-0.5477712	1.7548226	1.9029412
C	2.0789481	1.9242326	0.8769412
C	1.1403188	1.7026565	-1.9090588
N	-1.6541887	1.4069646	-0.8760588
N	1.6541887	-1.4069646	-0.8760588
H	-0.7135270	2.8005458	2.1839412
H	-0.1089901	-1.3019245	2.6469412
H	-1.5078918	1.2302099	1.9389412
H	0.7135270	-2.8005458	2.1839412
H	0.1089901	1.3019245	2.6469412
H	1.5078918	-1.2302099	1.9389412
H	-2.3987199	1.7227151	-0.2610588
H	1.7489777	-1.8768061	-1.7730588
H	-1.7489777	1.8768061	-1.7730588
H	2.3987199	-1.7227151	-0.2610588
H	-0.6284426	-1.0327962	-2.6100588
H	2.2097118	1.4694515	-1.9330588
H	0.6284426	1.0327962	-2.6100588
H	-1.0456082	-2.7214989	-2.3010588
H	-2.2097118	-1.4694515	-1.9330588
H	1.0456082	2.7214989	-2.3010588
H	-2.3745443	-0.9737275	1.3269412
H	2.8244182	2.2404845	0.1469412
H	-2.8244182	-2.2404845	0.1469412
H	1.9936975	2.6690905	1.6679412
H	2.3745443	0.9737275	1.3269412
H	-1.9936975	-2.6690905	1.6679412
H	-1.7695047	0.4037696	-1.0320588
H	1.7695047	-0.4037696	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 3.6 Å

Au	-0.2991525	-1.7749670	0.0039412
Au	0.2991525	1.7749670	0.0039412
C	-1.1560961	-1.8018295	-1.9090588
C	-2.0946158	-2.0238698	0.8769412
C	0.5320194	-1.8531607	1.9029412
C	-0.5320194	1.8531607	1.9029412
C	2.0946158	2.0238698	0.8769412
C	1.1560961	1.8018295	-1.9090588
N	-1.6382648	1.5047556	-0.8760588
N	1.6382648	-1.5047556	-0.8760588
H	-0.6982924	2.8988018	2.1839412
H	-0.1249658	-1.4005875	2.6469412
H	-1.4918805	1.3280733	1.9389412
H	0.6982924	-2.8988018	2.1839412
H	0.1249658	1.4005875	2.6469412
H	1.4918805	-1.3280733	1.9389412
H	-2.3829520	1.8201378	-0.2610588
H	1.7332861	-1.9745502	-1.7730588
H	-1.7332861	1.9745502	-1.7730588
H	2.3829520	-1.8201378	-0.2610588
H	-0.6445513	-1.1317162	-2.6100588
H	2.2256044	1.5691534	-1.9330588
H	0.6445513	1.1317162	-2.6100588
H	-1.0608817	-2.8206250	-2.3010588
H	-2.2256044	-1.5691534	-1.9330588
H	1.0608817	2.8206250	-2.3010588
H	-2.3906820	-1.0735110	1.3269412
H	2.8399294	2.3404904	0.1469412
H	-2.8399294	-2.3404904	0.1469412
H	2.0089968	2.7686855	1.6679412
H	2.3906820	1.0735110	1.3269412
H	-2.0089968	-2.7686855	1.6679412
H	-1.7530846	0.5015037	-1.0320588
H	1.7530846	-0.5015037	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 3.8 Å

Au	-0.3149050	-1.8737222	0.0039412
Au	0.3149050	1.8737222	0.0039412
C	-1.1718361	-1.9009813	-1.9090588
C	-2.1102529	-2.1234559	0.8769412
C	0.5163030	-1.9515313	1.9029412
C	-0.5163030	1.9515313	1.9029412
C	2.1102529	2.1234559	0.8769412
C	1.1718361	1.9009813	-1.9090588
N	-1.6223870	1.6026142	-0.8760588
N	1.6223870	-1.6026142	-0.8760588
H	-0.6830598	2.9970953	2.1839412
H	-0.1408915	-1.4992622	2.6469412
H	-1.4759209	1.4259997	1.9389412
H	0.6830598	-2.9970953	2.1839412
H	0.1408915	1.4992622	2.6469412
H	1.4759209	-1.4259997	1.9389412
H	-2.3672201	1.9176518	-0.2610588
H	1.7176257	-2.0723648	-1.7730588
H	-1.7176257	2.0723648	-1.7730588
H	2.3672201	-1.9176518	-0.2610588
H	-0.6606015	-1.2306313	-2.6100588
H	2.2414519	1.6688002	-1.9330588
H	0.6606015	1.2306313	-2.6100588
H	-1.0761502	-2.9197326	-2.3010588
H	-2.2414519	-1.6688002	-1.9330588
H	1.0761502	2.9197326	-2.3010588
H	-2.4067589	-1.1732342	1.3269412
H	2.8554199	2.4404214	0.1469412
H	-2.8554199	-2.4404214	0.1469412
H	2.0242893	2.8682319	1.6679412
H	2.4067589	1.1732342	1.3269412
H	-2.0242893	-2.8682319	1.6679412
H	-1.7367426	0.5993093	-1.0320588
H	1.7367426	-0.5993093	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 4.0 Å

Au	-0.3306268	-1.9724822	0.0039412
Au	0.3306268	1.9724822	0.0039412
C	-1.1875460	-2.0001115	-1.9090588
C	-2.1258666	-2.2229915	0.8769412
C	0.5006148	-2.0499321	1.9029412
C	-0.5006148	2.0499321	1.9029412
C	2.1258666	2.2229915	0.8769412
C	1.1875460	2.0001115	-1.9090588
N	-1.6065480	1.7005372	-0.8760588
N	1.6065480	-1.7005372	-0.8760588
H	-0.6678234	3.0954240	2.1839412
H	-0.1567751	-1.5979470	2.6469412
H	-1.4600056	1.5239860	1.9389412
H	0.6678234	-3.0954240	2.1839412
H	0.1567751	1.5979470	2.6469412
H	1.4600056	-1.5239860	1.9389412
H	-2.3515171	2.0152530	-0.2610588
H	1.7019896	-2.1702466	-1.7730588
H	-1.7019896	2.1702466	-1.7730588
H	2.3515171	-2.0152530	-0.2610588
H	-0.6766011	-1.3295407	-2.6100588
H	2.2572620	1.7683925	-1.9330588
H	0.6766011	1.3295407	-2.6100588
H	-1.0914200	-3.0188214	-2.3010588
H	-2.2572620	-1.7683925	-1.9330588
H	1.0914200	3.0188214	-2.3010588
H	-2.4227831	-1.2728981	1.3269412
H	2.8708966	2.5402789	0.1469412
H	-2.8708966	-2.5402789	0.1469412
H	2.0395812	2.9677303	1.6679412
H	2.4227831	1.2728981	1.3269412
H	-2.0395812	-2.9677303	1.6679412
H	-1.7204700	0.6971830	-1.0320588
H	1.7204700	-0.6971830	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 4.2 Å

Au	-0.3463240	-2.0712459	0.0039412
Au	0.3463240	2.0712459	0.0039412
C	-1.2032321	-2.0992204	-1.9090588
C	-2.1414628	-2.3224782	0.8769412
C	0.4849486	-2.1483611	1.9029412
C	-0.4849486	2.1483611	1.9029412
C	2.1414628	2.3224782	0.8769412
C	1.2032321	2.0992204	-1.9090588
N	-1.5907410	1.7985209	-0.8760588
N	1.5907410	-1.7985209	-0.8760588
H	-0.6525782	3.1937856	2.1839412
H	-0.1726232	-1.6966408	2.6469412
H	-1.4441276	1.6220287	1.9389412
H	0.6525782	-3.1937856	2.1839412
H	0.1726232	1.6966408	2.6469412
H	1.4441276	-1.6220287	1.9389412
H	-2.3358368	2.1129366	-0.2610588
H	1.6863718	-2.2681918	-1.7730588
H	-1.6863718	2.2681918	-1.7730588
H	2.3358368	-2.1129366	-0.2610588
H	-0.6925572	-1.4284438	-2.6100588
H	2.2730413	1.8679322	-1.9330588
H	0.6925572	1.4284438	-2.6100588
H	-1.1066958	-3.1178914	-2.3010588
H	-2.2730413	-1.8679322	-1.9330588
H	1.1066958	3.1178914	-2.3010588
H	-2.4387619	-1.3725044	1.3269412
H	2.8863650	2.6400656	0.1469412
H	-2.8863650	-2.6400656	0.1469412
H	2.0548775	3.0671822	1.6679412
H	2.4387619	1.3725044	1.3269412
H	-2.0548775	-3.0671822	1.6679412
H	-1.7042590	0.7951208	-1.0320588
H	1.7042590	-0.7951208	-1.0320588

$R(Au^{III}\cdots Au^{III})$ = 4.4 Å

Au	-0.3620022	-2.1700125	0.0039412
Au	0.3620022	2.1700125	0.0039412
C	-1.2188997	-2.1983082	-1.9090588
C	-2.1570467	-2.4219178	0.8769412
C	0.4692994	-2.2468161	1.9029412
C	-0.4692994	2.2468161	1.9029412
C	2.1570467	2.4219178	0.8769412
C	1.2188997	2.1983082	-1.9090588
N	-1.5749605	1.8965613	-0.8760588
N	1.5749605	-1.8965613	-0.8760588
H	-0.6373209	3.2921776	2.1839412
H	-0.1884418	-1.7953423	2.6469412
H	-1.4282809	1.7201241	1.9389412
H	0.6373209	-3.2921776	2.1839412
H	0.1884418	1.7953423	2.6469412
H	1.4282809	-1.7201241	1.9389412
H	-2.3201741	2.2106977	-0.2610588
H	1.6707674	-2.3661964	-1.7730588
H	-1.6707674	2.3661964	-1.7730588
H	2.3201741	-2.2106977	-0.2610588
H	-0.7084763	-1.5273403	-2.6100588
H	2.2887955	1.9674211	-1.9330588
H	0.7084763	1.5273403	-2.6100588
H	-1.1219815	-3.2169430	-2.3010588
H	-2.2887955	-1.9674211	-1.9330588
H	1.1219815	3.2169430	-2.3010588
H	-2.4547018	-1.4720555	1.3269412
H	2.9018297	2.7397844	0.1469412
H	-2.9018297	-2.7397844	0.1469412
H	2.0701822	3.1665892	1.6679412
H	2.4547018	1.4720555	1.3269412
H	-2.0701822	-3.1665892	1.6679412
H	-1.6881023	0.8931188	-1.0320588
H	1.6881023	-0.8931188	-1.0320588

6. Cartesian coordinates of molecule *2*.

Au	0.1866268	-1.5365107	-0.0029950
N	-0.5780727	-1.9576709	-1.8102537
N	1.1366838	-1.1267214	1.7408085
N	0.5632619	-1.4579206	2.7651548
N	-2.4449519	-1.7163414	0.9394250
N	-1.7822505	-2.1406922	-1.8905681
N	-1.3729930	-2.3051820	1.0014100
N	1.8911514	-0.8877992	-0.8952554
N	1.9235083	-0.9140363	-2.1142901
N	-2.9163105	-2.3328916	-2.1006468
N	2.0689890	-0.8946993	-3.2750239
N	0.1071488	-1.7315756	3.8074700
N	-3.5219527	-1.2706566	0.9679769
Au	-0.1866268	1.5365107	-0.0029950
N	1.3729930	2.3051820	1.0014100
N	2.4449519	1.7163414	0.9394250
N	1.7822505	2.1406922	-1.8905681
N	-1.1366838	1.1267214	1.7408085
N	-1.9235083	0.9140363	-2.1142901
N	-0.5632619	1.4579206	2.7651548
N	-1.8911514	0.8877992	-0.8952554
N	0.5780727	1.9576709	-1.8102537
N	3.5219527	1.2706566	0.9679769
N	-2.0689890	0.8946993	-3.2750239
N	2.9163105	2.3328916	-2.1006468
N	-0.1071488	1.7315756	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 2.8 Å

Au	0.1876907	-1.3873616	-0.0029950
N	-0.5712103	-1.8188827	-1.8102537
N	1.1320868	-0.9646896	1.7408085
N	0.5632222	-1.3036565	2.7651548
N	-2.4411989	-1.6029649	0.9394250
N	-1.7727877	-2.0182637	-1.8905681
N	-1.3613310	-2.1771725	1.0014100
N	1.8832353	-0.7155288	-0.8952554
N	1.9159460	-0.7413234	-2.1142901
N	-2.9041289	-2.2258684	-2.1006468
N	2.0611503	-0.7200096	-3.2750239
N	0.1108729	-1.5834893	3.8074700
N	-3.5241614	-1.1719684	0.9679769
Au	-0.1876907	1.3873616	-0.0029950
N	1.3613310	2.1771725	1.0014100
N	2.4411989	1.6029649	0.9394250
N	1.7727877	2.0182637	-1.8905681
N	-1.1320868	0.9646896	1.7408085
N	-1.9159460	0.7413234	-2.1142901
N	-0.5632222	1.3036565	2.7651548
N	-1.8832353	0.7155288	-0.8952554
N	0.5712103	1.8188827	-1.8102537
N	3.5241614	1.1719684	0.9679769
N	-2.0611503	0.7200096	-3.2750239
N	2.9041289	2.2258684	-2.1006468
N	-0.1108729	1.5834893	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 3.0 Å

Au	0.1872436	-1.4882674	-0.0029950
N	-0.5756436	-1.9127014	-1.8102537
N	1.1355355	-1.0744098	1.7408085
N	0.5635385	-1.4080637	2.7651548
N	-2.4435401	-1.6793760	0.9394250
N	-1.7790259	-2.1008824	-1.8905681
N	-1.3690671	-2.2636165	1.0014100
N	1.8889721	-0.8322559	-0.8952554
N	1.9214412	-0.8583541	-2.1142901
N	-2.9122517	-2.2979408	-2.1006468
N	2.0668376	-0.8383936	-3.2750239
N	0.1086024	-1.6836711	3.8074700
N	-3.5224412	-1.2383115	0.9679769
Au	-0.1872436	1.4882674	-0.0029950
N	1.3690671	2.2636165	1.0014100
N	2.4435401	1.6793760	0.9394250
N	1.7790259	2.1008824	-1.8905681
N	-1.1355355	1.0744098	1.7408085
N	-1.9214412	0.8583541	-2.1142901
N	-0.5635385	1.4080637	2.7651548
N	-1.8889721	0.8322559	-0.8952554
N	0.5756436	1.9127014	-1.8102537
N	3.5224412	1.2383115	0.9679769
N	-2.0668376	0.8383936	-3.2750239
N	2.9122517	2.2979408	-2.1006468
N	-0.1086024	1.6836711	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 3.2 Å

Au	0.1856846	-1.5891889	0.0636810
N	-0.5809251	-2.0068620	-1.7435778
N	1.1375981	-1.1837308	1.8074845
N	0.5626738	-1.5123149	2.8318308
N	-2.4466858	-1.7570326	1.0061010
N	-1.7859239	-2.1843971	-1.8238921
N	-1.3774198	-2.3507491	1.0680860
N	1.8931460	-0.9482471	-0.8285794
N	1.9253831	-0.9746313	-2.0476141
N	-2.9208475	-2.3714296	-2.0339708
N	2.0709503	-0.9559570	-3.2083479
N	0.1053190	-1.7838897	3.8741460
N	-3.5216456	-1.3064473	1.0346529
Au	-0.1856846	1.5891889	0.0636810
N	1.3774198	2.3507491	1.0680860
N	2.4466858	1.7570326	1.0061010
N	1.7859239	2.1843971	-1.8238921
N	-1.1375981	1.1837308	1.8074845
N	-1.9253831	0.9746313	-2.0476141
N	-0.5626738	1.5123149	2.8318308
N	-1.8931460	0.9482471	-0.8285794
N	0.5809251	2.0068620	-1.7435778
N	3.5216456	1.3064473	1.0346529
N	-2.0709503	0.9559570	-3.2083479
N	2.9208475	2.3714296	-2.0339708
N	-0.1053190	1.7838897	3.8741460

$R(Au^{III}\cdots Au^{III})$ = 3.4 Å

Au	0.1831768	-1.6901024	-0.0029950
N	-0.5868954	-2.1013566	-1.8102537
N	1.1384444	-1.2926110	1.7408085
N	0.5607951	-1.6163806	2.7651548
N	-2.4505039	-1.8359489	0.9394250
N	-1.7933354	-2.2688187	-1.8905681
N	-1.3862352	-2.4385776	1.0014100
N	1.8959332	-1.0634476	-0.8952554
N	1.9279487	-1.0901001	-2.1142901
N	-2.9297818	-2.4463632	-2.1006468
N	2.0736669	-1.0726426	-3.2750239
N	0.1011874	-1.8841251	3.8074700
N	-3.5216619	-1.3763989	0.9679769
Au	-0.1831768	1.6901024	-0.0029950
N	1.3862352	2.4385776	1.0014100
N	2.4505039	1.8359489	0.9394250
N	1.7933354	2.2688187	-1.8905681
N	-1.1384444	1.2926110	1.7408085
N	-1.9279487	1.0901001	-2.1142901
N	-0.5607951	1.6163806	2.7651548
N	-1.8959332	1.0634476	-0.8952554
N	0.5868954	2.1013566	-1.8102537
N	3.5216619	1.3763989	0.9679769
N	-2.0736669	1.0726426	-3.2750239
N	2.9297818	2.4463632	-2.1006468
N	-0.1011874	1.8841251	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 3.6 Å

Au	0.1798705	-1.7909904	-0.0029950
N	-0.5934127	-2.1961748	-1.8102537
N	1.1382350	-1.4010249	1.7408085
N	0.5580569	-1.7202410	2.7651548
N	-2.4548760	-1.9161172	0.9394250
N	-1.8011325	-2.3541425	-1.8905681
N	-1.3953802	-2.5270982	1.0014100
N	1.8975028	-1.1778266	-0.8952554
N	1.9293077	-1.2047302	-2.1142901
N	-2.9389403	-2.5227429	-2.1006468
N	2.0751587	-1.1884193	-3.2750239
N	0.0963575	-1.9843622	3.8074700
N	-3.5223862	-1.4481562	0.9679769
Au	-0.1798705	1.7909904	-0.0029950
N	1.3953802	2.5270982	1.0014100
N	2.4548760	1.9161172	0.9394250
N	1.8011325	2.3541425	-1.8905681
N	-1.1382350	1.4010249	1.7408085
N	-1.9293077	1.2047302	-2.1142901
N	-0.5580569	1.7202410	2.7651548
N	-1.8975028	1.1778266	-0.8952554
N	0.5934127	2.1961748	-1.8102537
N	3.5223862	1.4481562	0.9679769
N	-2.0751587	1.1884193	-3.2750239
N	2.9389403	2.5227429	-2.1006468
N	-0.0963575	1.9843622	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 3.8 Å

Au	0.1759016	-1.8918400	-0.0029950
N	-0.6003518	-2.2913046	-1.8102537
N	1.1371189	-1.5089602	1.7408085
N	0.5546000	-1.8238845	2.7651548
N	-2.4596968	-1.9975124	0.9394250
N	-1.8092049	-2.4403520	-1.8905681
N	-1.4047405	-2.6162985	1.0014100
N	1.8980138	-1.2913733	-0.8952554
N	1.9296192	-1.3185110	-2.1142901
N	-2.9482264	-2.6005479	-2.1006468
N	2.0755866	-1.3032773	-3.2750239
N	0.0909633	-2.0845900	3.8074700
N	-3.5237233	-1.5216833	0.9679769
Au	-0.1759016	1.8918400	-0.0029950
N	1.4047405	2.6162985	1.0014100
N	2.4596968	1.9975124	0.9394250
N	1.8092049	2.4403520	-1.8905681
N	-1.1371189	1.5089602	1.7408085
N	-1.9296192	1.3185110	-2.1142901
N	-0.5546000	1.8238845	2.7651548
N	-1.8980138	1.2913733	-0.8952554
N	0.6003518	2.2913046	-1.8102537
N	3.5237233	1.5216833	0.9679769
N	-2.0755866	1.3032773	-3.2750239
N	2.9482264	2.6005479	-2.1006468
N	-0.0909633	2.0845900	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 4.0 Å

Au	0.1713915	-1.9926427	-0.0029950
N	-0.6076042	-2.3867327	-1.8102537
N	1.1352321	-1.6164155	1.7408085
N	0.5505506	-1.9273062	2.7651548
N	-2.4648743	-2.0800966	0.9394250
N	-1.8174585	-2.5274216	-1.8905681
N	-1.4142198	-2.7061593	1.0014100
N	1.8976128	-1.4040927	-0.8952554
N	1.9290299	-1.4314481	-2.1142901
N	-2.9575600	-2.6797413	-2.1006468
N	2.0750991	-1.4172237	-3.2750239
N	0.0851232	-2.1848010	3.8074700
N	-3.5255866	-1.5969249	0.9679769
Au	-0.1713915	1.9926427	-0.0029950
N	1.4142198	2.7061593	1.0014100
N	2.4648743	2.0800966	0.9394250
N	1.8174585	2.5274216	-1.8905681
N	-1.1352321	1.6164155	1.7408085
N	-1.9290299	1.4314481	-2.1142901
N	-0.5505506	1.9273062	2.7651548
N	-1.8976128	1.4040927	-0.8952554
N	0.6076042	2.3867327	-1.8102537
N	3.5255866	1.5969249	0.9679769
N	-2.0750991	1.4172237	-3.2750239
N	2.9575600	2.6797413	-2.1006468
N	-0.0851232	2.1848010	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 4.2 Å

Au	0.1664475	-2.0933932	-0.0029950
N	-0.6150766	-2.4824451	-1.8102537
N	1.1326973	-1.7233974	1.7408085
N	0.5460205	-2.0305063	2.7651548
N	-2.4703280	-2.1638229	0.9394250
N	-1.8258142	-2.6153189	-1.8905681
N	-1.4237380	-2.7966566	1.0014100
N	1.8964330	-1.5160017	-0.8952554
N	1.9276728	-1.5435595	-2.1142901
N	-2.9668754	-2.7602738	-2.1006468
N	2.0738308	-1.5302785	-3.2750239
N	0.0789401	-2.2849905	3.8074700
N	-3.5278984	-1.6738122	0.9679769
Au	-0.1664475	2.0933932	-0.0029950
N	1.4237380	2.7966566	1.0014100
N	2.4703280	2.1638229	0.9394250
N	1.8258142	2.6153189	-1.8905681
N	-1.1326973	1.7233974	1.7408085
N	-1.9276728	1.5435595	-2.1142901
N	-0.5460205	2.0305063	2.7651548
N	-1.8964330	1.5160017	-0.8952554
N	0.6150766	2.4824451	-1.8102537
N	3.5278984	1.6738122	0.9679769
N	-2.0738308	1.5302785	-3.2750239
N	2.9668754	2.7602738	-2.1006468
N	-0.0789401	2.2849905	3.8074700

$R(Au^{III}\cdots Au^{III})$ = 4.4 Å

Au	0.1611629	-2.1940890	-0.0029950
N	-0.6226900	-2.5784272	-1.8102537
N	1.1296235	-1.8299190	1.7408085
N	0.5411078	-2.1334891	2.7651548
N	-2.4759890	-2.2486378	0.9394250
N	-1.8342058	-2.7040071	-1.8905681
N	-1.4332290	-2.8877630	1.0014100
N	1.8945943	-1.6271265	-0.8952554
N	1.9256676	-1.6548719	-2.1142901
N	-2.9761193	-2.8420875	-2.1006468
N	2.0719029	-1.6424714	-3.2750239
N	0.0725033	-2.3851558	3.8074700
N	-3.5305891	-1.7522670	0.9679769
Au	-0.1611629	2.1940890	-0.0029950
N	1.4332290	2.8877630	1.0014100
N	2.4759890	2.2486378	0.9394250
N	1.8342058	2.7040071	-1.8905681
N	-1.1296235	1.8299190	1.7408085
N	-1.9256676	1.6548719	-2.1142901
N	-0.5411078	2.1334891	2.7651548
N	-1.8945943	1.6271265	-0.8952554
N	0.6226900	2.5784272	-1.8102537
N	3.5305891	1.7522670	0.9679769
N	-2.0719029	1.6424714	-3.2750239
N	2.9761193	2.8420875	-2.1006468
N	-0.0725033	2.3851558	3.8074700

7. Cartesian coordinates of molecule *3*.

Au	-0.1265006	-1.6819570	0.0009972
Au	0.1265006	1.6819570	0.0009972
N	1.2119386	-2.3554747	-1.5749130
C	-1.5130303	-1.2193849	-1.3916588
C	-1.4886569	-1.1963392	1.4102227
C	1.4886569	1.1963392	1.4102227
C	1.5130303	1.2193849	-1.3916588
N	-1.2119386	2.3554747	-1.5749130
N	-1.2425384	2.3538906	1.5552478
N	1.2425384	-2.3538906	1.5552478
H	2.1123159	2.0777093	1.5730196
H	-2.1248220	-0.3709117	1.1010378
H	0.9589881	0.9449567	2.3308182
H	-2.1123159	-2.0777093	1.5730196
H	2.1248220	0.3709117	1.1010378
H	-0.9589881	-0.9449567	2.3308182
H	-1.4016517	1.6414678	2.2668473
H	0.8271755	-3.1505684	2.0414160
H	-0.8271755	3.1505684	2.0414160
H	1.4016517	-1.6414678	2.2668473
H	2.0943067	-1.8484550	-1.6423713
H	-0.7638038	2.2688994	-2.4873060
H	-2.0943067	1.8484550	-1.6423713
H	1.4504265	-3.3439561	-1.4815414
H	0.7638038	-2.2688994	-2.4873060
H	-1.4504265	3.3439561	-1.4815414
H	-2.3605078	-0.6758338	-0.9817082
H	1.0284977	0.6373129	-2.1772947
H	-1.0284977	-0.6373129	-2.1772947
H	1.8699137	2.1674862	-1.8005517
H	2.3605078	0.6758338	-0.9817082
H	-1.8699137	-2.1674862	-1.8005517
H	-2.1667355	2.6612539	1.2526848
H	2.1667355	-2.6612539	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 2.8 Å

Au	-0.1045103	-1.3960937	0.0009972
Au	0.1045103	1.3960937	0.0009972
N	1.2341640	-2.0691439	-1.5749130
C	-1.4912015	-0.9340059	-1.3916588
C	-1.4668362	-0.9109517	1.4102227
C	1.4668362	0.9109517	1.4102227
C	1.4912015	0.9340059	-1.3916588
N	-1.2341640	2.0691439	-1.5749130
N	-1.2647633	2.0675491	1.5552478
N	1.2647633	-2.0675491	1.5552478
H	2.0901873	1.7925395	1.5730196
H	-2.1032895	-0.0857464	1.1010378
H	0.9372552	0.6593842	2.3308182
H	-2.0901873	-1.7925395	1.5730196
H	2.1032895	0.0857464	1.1010378
H	-0.9372552	-0.6593842	2.3308182
H	-1.4236277	1.3550707	2.2668473
H	0.8496787	-2.8643719	2.0414160
H	-0.8496787	2.8643719	2.0414160
H	1.4236277	-1.3550707	2.2668473
H	2.1163550	-1.5618160	-1.6423713
H	-0.7859990	1.9827251	-2.4873060
H	-2.1163550	1.5618160	-1.6423713
H	1.4729972	-3.0575419	-1.4815414
H	0.7859990	-1.9827251	-2.4873060
H	-1.4729972	3.0575419	-1.4815414
H	-2.3388688	-0.3907508	-0.9817082
H	1.0068722	0.3517647	-2.1772947
H	-1.0068722	-0.3517647	-2.1772947
H	1.8477537	1.8822318	-1.8005517
H	2.3388688	0.3907508	-0.9817082
H	-1.8477537	-1.8822318	-1.8005517
H	-2.1890676	2.3745896	1.2526848
H	2.1890676	-2.3745896	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 3.0 Å

Au	-0.1121680	-1.4958002	0.0009972
Au	0.1121680	1.4958002	0.0009972
N	1.2264196	-2.1690228	-1.5749130
C	-1.4987997	-1.0335338	-1.3916588
C	-1.4744314	-1.0104827	1.4102227
C	1.4744314	1.0104827	1.4102227
C	1.4987997	1.0335338	-1.3916588
N	-1.2264196	2.1690228	-1.5749130
N	-1.2570191	2.1674320	1.5552478
N	1.2570191	-2.1674320	1.5552478
H	2.0978960	1.8919903	1.5730196
H	-2.1107784	-0.1851955	1.1010378
H	0.9448180	0.7589835	2.3308182
H	-2.0978960	-1.8919903	1.5730196
H	2.1107784	0.1851955	1.1010378
H	-0.9448180	-0.7589835	2.3308182
H	-1.4159753	1.4549741	2.2668473
H	0.8418319	-2.9642013	2.0414160
H	-0.8418319	2.9642013	2.0414160
H	1.4159753	-1.4549741	2.2668473
H	2.1086760	-1.6618086	-1.6423713
H	-0.7782658	2.0825464	-2.4873060
H	-2.1086760	1.6618086	-1.6423713
H	1.4651255	-3.1574516	-1.4815414
H	0.7782658	-2.0825464	-2.4873060
H	-1.4651255	3.1574516	-1.4815414
H	-2.3463970	-0.4901696	-0.9817082
H	1.0143954	0.4513550	-2.1772947
H	-1.0143954	-0.4513550	-2.1772947
H	1.8554740	1.9817138	-1.8005517
H	2.3463970	0.4901696	-0.9817082
H	-1.8554740	-1.9817138	-1.8005517
H	-2.1812839	2.4745915	1.2526848
H	2.1812839	-2.4745915	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 3.2 Å

Au	-0.1198402	-1.5955057	0.0009972
Au	0.1198402	1.5955057	0.0009972
N	1.2186654	-2.2688913	-1.5749130
C	-1.5064156	-1.1330704	-1.3916588
C	-1.4820445	-1.1100223	1.4102227
C	1.4820445	1.1100223	1.4102227
C	1.5064156	1.1330704	-1.3916588
N	-1.2186654	2.2688913	-1.5749130
N	-1.2492651	2.2673042	1.5552478
N	1.2492651	-2.2673042	1.5552478
H	2.1056164	1.9914539	1.5730196
H	-2.1182909	-0.2846576	1.1010378
H	0.9524004	0.8585875	2.3308182
H	-2.1056164	-1.9914539	1.5730196
H	2.1182909	0.2846576	1.1010378
H	-0.9524004	-0.8585875	2.3308182
H	-1.4083081	1.5548656	2.2668473
H	0.8339809	-3.0640229	2.0414160
H	-0.8339809	3.0640229	2.0414160
H	1.4083081	-1.5548656	2.2668473
H	2.1009835	-1.7617845	-1.6423713
H	-0.7705221	2.1823602	-2.4873060
H	-2.1009835	1.7617845	-1.6423713
H	1.4572509	-3.2573491	-1.4815414
H	0.7705221	-2.1823602	-2.4873060
H	-1.4572509	3.2573491	-1.4815414
H	-2.3539467	-0.5896029	-0.9817082
H	1.0219404	0.5509505	-2.1772947
H	-1.0219404	-0.5509505	-2.1772947
H	1.8632054	2.0812069	-1.8005517
H	2.3539467	0.5896029	-0.9817082
H	-1.8632054	-2.0812069	-1.8005517
H	-2.1734925	2.5745763	1.2526848
H	2.1734925	-2.5745763	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 3.4 Å

Au	-0.1275254	-1.6952101	0.0009972
Au	0.1275254	1.6952101	0.0009972
N	1.2109027	-2.3687498	-1.5749130
C	-1.5140475	-1.2326152	-1.3916588
C	-1.4896738	-1.2095699	1.4102227
C	1.4896738	1.2095699	1.4102227
C	1.5140475	1.2326152	-1.3916588
N	-1.2109027	2.3687498	-1.5749130
N	-1.2415026	2.3671663	1.5552478
N	1.2415026	-2.3671663	1.5552478
H	2.1133472	2.0909297	1.5730196
H	-2.1258252	-0.3841319	1.1010378
H	0.9600008	0.9581961	2.3308182
H	-2.1133472	-2.0909297	1.5730196
H	2.1258252	0.3841319	1.1010378
H	-0.9600008	-0.9581961	2.3308182
H	-1.4006276	1.6547460	2.2668473
H	0.8261265	-3.1638372	2.0414160
H	-0.8261265	3.1638372	2.0414160
H	1.4006276	-1.6547460	2.2668473
H	2.0932792	-1.8617447	-1.6423713
H	-0.7627693	2.2821672	-2.4873060
H	-2.0932792	1.8617447	-1.6423713
H	1.4493744	-3.3572351	-1.4815414
H	0.7627693	-2.2821672	-2.4873060
H	-1.4493744	3.3572351	-1.4815414
H	-2.3615161	-0.6890501	-0.9817082
H	1.0295053	0.6505511	-2.1772947
H	-1.0295053	-0.6505511	-2.1772947
H	1.8709465	2.1807106	-1.8005517
H	2.3615161	0.6890501	-0.9817082
H	-1.8709465	-2.1807106	-1.8005517
H	-2.1656945	2.6745448	1.2526848
H	2.1656945	-2.6745448	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 3.6 Å

Au	-0.1352223	-1.7949136	0.0009972
Au	0.1352223	1.7949136	0.0009972
N	1.2031325	-2.4685991	-1.5749130
C	-1.5216940	-1.3321678	-1.3916588
C	-1.4973178	-1.3091251	1.4102227
C	1.4973178	1.3091251	1.4102227
C	1.5216940	1.3321678	-1.3916588
N	-1.2031325	2.4685991	-1.5749130
N	-1.2337325	2.4670188	1.5552478
N	1.2337325	-2.4670188	1.5552478
H	2.1210872	2.1904170	1.5730196
H	-2.1333794	-0.4836179	1.1010378
H	0.9676174	1.0578090	2.3308182
H	-2.1210872	-2.1904170	1.5730196
H	2.1333794	0.4836179	1.1010378
H	-0.9676174	-1.0578090	2.3308182
H	-1.3929351	1.7546159	2.2668473
H	0.8182698	-3.2636445	2.0414160
H	-0.8182698	3.2636445	2.0414160
H	1.3929351	-1.7546159	2.2668473
H	2.0855641	-1.9616899	-1.6423713
H	-0.7550086	2.3819676	-2.4873060
H	-2.0855641	1.9616899	-1.6423713
H	1.4414965	-3.4571103	-1.4815414
H	0.7550086	-2.3819676	-2.4873060
H	-1.4414965	3.4571103	-1.4815414
H	-2.3691034	-0.7885104	-0.9817082
H	1.0370885	0.7501565	-2.1772947
H	-1.0370885	-0.7501565	-2.1772947
H	1.8786962	2.2802244	-1.8005517
H	2.3691034	0.7885104	-0.9817082
H	-1.8786962	-2.2802244	-1.8005517
H	-2.1578910	2.7744979	1.2526848
H	2.1578910	-2.7744979	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 3.8 Å

Au	-0.1429296	-1.8946164	0.0009972
Au	0.1429296	1.8946164	0.0009972
N	1.1953558	-2.5684396	-1.5749130
C	-1.5293538	-1.4317278	-1.3916588
C	-1.5049751	-1.4086876	1.4102227
C	1.5049751	1.4086876	1.4102227
C	1.5293538	1.4317278	-1.3916588
N	-1.1953558	2.5684396	-1.5749130
N	-1.2259560	2.5668624	1.5552478
N	1.2259560	-2.5668624	1.5552478
H	2.1288352	2.2899153	1.5730196
H	-2.1409517	-0.5831150	1.1010378
H	0.9752489	1.1574261	2.3308182
H	-2.1288352	-2.2899153	1.5730196
H	2.1409517	0.5831150	1.1010378
H	-0.9752489	-1.1574261	2.3308182
H	-1.3852318	1.8544759	2.2668473
H	0.8104112	-3.3634453	2.0414160
H	-0.8104112	3.3634453	2.0414160
H	1.3852318	-1.8544759	2.2668473
H	2.0778396	-2.0616212	-1.6423713
H	-0.7472408	2.4817620	-2.4873060
H	-2.0778396	2.0616212	-1.6423713
H	1.4336181	-3.5569753	-1.4815414
H	0.7472408	-2.4817620	-2.4873060
H	-1.4336181	3.5569753	-1.4815414
H	-2.3767072	-0.8879832	-0.9817082
H	1.0446883	0.8497664	-2.1772947
H	-1.0446883	-0.8497664	-2.1772947
H	1.8864535	2.3797476	-1.8005517
H	2.3767072	0.8879832	-0.9817082
H	-1.8864535	-2.3797476	-1.8005517
H	-2.1500828	2.8744367	1.2526848
H	2.1500828	-2.8744367	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 4.0 Å

Au	-0.1506464	-1.9943183	0.0009972
Au	0.1506464	1.9943183	0.0009972
N	1.1875734	-2.6682718	-1.5749130
C	-1.5370255	-1.5312948	-1.3916588
C	-1.5126446	-1.5082570	1.4102227
C	1.5126446	1.5082570	1.4102227
C	1.5370255	1.5312948	-1.3916588
N	-1.1875734	2.6682718	-1.5749130
N	-1.2181738	2.6666977	1.5552478
N	1.2181738	-2.6666977	1.5552478
H	2.1365905	2.3894240	1.5730196
H	-2.1485408	-0.6826225	1.1010378
H	0.9828939	1.2570471	2.3308182
H	-2.1365905	-2.3894240	1.5730196
H	2.1485408	0.6826225	1.1010378
H	-0.9828939	-1.2570471	2.3308182
H	-1.3775190	1.9543267	2.2668473
H	0.8025515	-3.4632401	2.0414160
H	-0.8025515	3.4632401	2.0414160
H	1.3775190	-1.9543267	2.2668473
H	2.0701066	-2.1615394	-1.6423713
H	-0.7394669	2.5815506	-2.4873060
H	-2.0701066	2.1615394	-1.6423713
H	1.4257395	-3.6568307	-1.4815414
H	0.7394669	-2.5815506	-2.4873060
H	-1.4257395	3.6568307	-1.4815414
H	-2.3843259	-0.9874678	-0.9817082
H	1.0523033	0.9493806	-2.1772947
H	-1.0523033	-0.9493806	-2.1772947
H	1.8942175	2.4792799	-1.8005517
H	2.3843259	0.9874678	-0.9817082
H	-1.8942175	-2.4792799	-1.8005517
H	-2.1422707	2.9743619	1.2526848
H	2.1422707	-2.9743619	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 4.2 Å

Au	-0.1583697	-2.0940198	0.0009972
Au	0.1583697	2.0940198	0.0009972
N	1.1797886	-2.7680954	-1.5749130
C	-1.5447065	-1.6308698	-1.3916588
C	-1.5203235	-1.6078343	1.4102227
C	1.5203235	1.6078343	1.4102227
C	1.5447065	1.6308698	-1.3916588
N	-1.1797886	2.7680954	-1.5749130
N	-1.2103891	2.7665240	1.5552478
N	1.2103891	-2.7665240	1.5552478
H	2.1443498	2.4889443	1.5730196
H	-2.1561445	-0.7821417	1.1010378
H	0.9905500	1.3566726	2.3308182
H	-2.1443498	-2.4889443	1.5730196
H	2.1561445	0.7821417	1.1010378
H	-0.9905500	-1.3566726	2.3308182
H	-1.3697993	2.0541675	2.2668473
H	0.7946942	-3.5630286	2.0414160
H	-0.7946942	3.5630286	2.0414160
H	1.3697993	-2.0541675	2.2668473
H	2.0623680	-2.2614435	-1.6423713
H	-0.7316900	2.6813333	-2.4873060
H	-2.0623680	2.2614435	-1.6423713
H	1.4178645	-3.7566760	-1.4815414
H	0.7316900	-2.6813333	-2.4873060
H	-1.4178645	3.7566760	-1.4815414
H	-2.3919574	-1.0869655	-0.9817082
H	1.0599313	1.0489998	-2.1772947
H	-1.0599313	-1.0489998	-2.1772947
H	1.9019851	2.5788223	-1.8005517
H	2.3919574	1.0869655	-0.9817082
H	-1.9019851	-2.5788223	-1.8005517
H	-2.1344579	3.0742725	1.2526848
H	2.1344579	-3.0742725	1.2526848

$R(Au^{III}\cdots Au^{III})$ = 4.4 Å

Au	-0.1661024	-2.1937206	0.0009972
Au	0.1661024	2.1937206	0.0009972
N	1.1719971	-2.8679128	-1.5749130
C	-1.5523988	-1.7304497	-1.3916588
C	-1.5280138	-1.7074163	1.4102227
C	1.5280138	1.7074163	1.4102227
C	1.5523988	1.7304497	-1.3916588
N	-1.1719971	2.8679128	-1.5749130
N	-1.2025978	2.8663441	1.5552478
N	1.2025978	-2.8663441	1.5552478
H	2.1521169	2.5884719	1.5730196
H	-2.1637628	-0.8816683	1.1010378
H	0.9982184	1.4563008	2.3308182
H	-2.1521169	-2.5884719	1.5730196
H	2.1637628	0.8816683	1.1010378
H	-0.9982184	-1.4563008	2.3308182
H	-1.3620701	2.1540015	2.2668473
H	0.7868334	-3.6628124	2.0414160
H	-0.7868334	3.6628124	2.0414160
H	1.3620701	-2.1540015	2.2668473
H	2.0546207	-2.3613379	-1.6423713
H	-0.7239060	2.7811117	-2.4873060
H	-2.0546207	2.3613379	-1.6423713
H	1.4099868	-3.8565142	-1.4815414
H	0.7239060	-2.7811117	-2.4873060
H	-1.4099868	3.8565142	-1.4815414
H	-2.3996023	-1.1864715	-0.9817082
H	1.0675729	1.1486220	-2.1772947
H	-1.0675729	-1.1486220	-2.1772947
H	1.9097600	2.6783711	-1.8005517
H	2.3996023	1.1864715	-0.9817082
H	-1.9097600	-2.6783711	-1.8005517
H	-2.1266398	3.1741732	1.2526848
H	2.1266398	-3.1741732	1.2526848

8. Cartesian coordinates of $[Au^{III}(CH_3)_3(NH_3)]\cdots[(CH_4)_3(NH_3)]_2$.

$R(Au^{III}\cdots Au^{III})$ = 3.48 Å

Au	-0.2929092	-1.7151689	0.0040000
C	-1.1499092	-1.7401689	-1.9090000
C	-2.0889092	-1.9601689	0.8770000
C	0.5380908	-1.7951689	1.9030000
C	-0.5380908	1.7951689	1.9030000
C	2.0889092	1.9601689	0.8770000
C	1.1499092	1.7401689	-1.9090000
N	-1.6450908	1.4491689	-0.8760000
N	1.6450908	-1.4491689	-0.8760000
H	-0.7020908	2.8411689	2.1840000
H	-0.1179092	-1.3411689	2.6470000
H	-1.4990908	1.2721689	1.9390000
H	0.7020908	-2.8411689	2.1840000
H	0.1179092	1.3411689	2.6470000
H	1.4990908	-1.2721689	1.9390000
H	-2.3890908	1.7661689	-0.2610000
H	1.7390908	-1.9191689	-1.7730000
H	-1.7390908	1.9191689	-1.7730000
H	2.3890908	-1.7661689	-0.2610000
H	-0.6369092	-1.0711689	-2.6100000
H	2.2189092	1.5051689	-1.9330000
H	0.6369092	1.0711689	-2.6100000
H	-1.0569092	-2.7591689	-2.3010000
H	-2.2189092	-1.5051689	-1.9330000
H	1.0569092	2.7591689	-2.3010000
H	-2.3829092	-1.0091689	1.3270000
H	2.8349092	2.2751689	0.1470000
H	-2.8349092	-2.2751689	0.1470000
H	2.0049092	2.7051689	1.6680000
H	2.3829092	1.0091689	1.3270000
H	-2.0049092	-2.7051689	1.6680000
H	-1.7620908	0.4461689	-1.0320000
H	1.7620908	-0.4461689	-1.0320000
H	-0.2531449	1.6929706	0.8856245
H	1.1609544	1.8746214	0.3973193
H	0.6293765	1.6268306	-0.9891146

$R(Au^{III}\cdots Au^{III})$ = 3.59 Å

Au	0.3021678	1.7693840	0.0040000
C	-1.1591678	-1.7943840	-1.9090000
C	-2.0981678	-2.0143840	0.8770000
C	0.5288322	-1.8493840	1.9030000
C	-0.5288322	1.8493840	1.9030000
C	2.0981678	2.0143840	0.8770000
C	1.1591678	1.7943840	-1.9090000
N	-1.6358322	1.5033840	-0.8760000
N	1.6358322	-1.5033840	-0.8760000
H	-0.6928322	2.8953840	2.1840000
H	-0.1271678	-1.3953840	2.6470000
H	-1.4898322	1.3263840	1.9390000
H	0.6928322	-2.8953840	2.1840000
H	0.1271678	1.3953840	2.6470000
H	1.4898322	-1.3263840	1.9390000
H	-2.3798322	1.8203840	-0.2610000
H	1.7298322	-1.9733840	-1.7730000
H	-1.7298322	1.9733840	-1.7730000
H	2.3798322	-1.8203840	-0.2610000
H	-0.6461678	-1.1253840	-2.6100000
H	2.2281678	1.5593840	-1.9330000
H	0.6461678	1.1253840	-2.6100000
H	-1.0661678	-2.8133840	-2.3010000
H	-2.2281678	-1.5593840	-1.9330000
H	1.0661678	2.8133840	-2.3010000
H	-2.3921678	-1.0633840	1.3270000
H	2.8441678	2.3293840	0.1470000
H	-2.8441678	-2.3293840	0.1470000
H	2.0141678	2.7593840	1.6680000
H	2.3921678	1.0633840	1.3270000
H	-2.0141678	-2.7593840	1.6680000
H	-1.7528322	0.5003840	-1.0320000
H	1.7528322	-0.5003840	-1.0320000
H	-1.1708326	-1.9297862	0.3961938
H	-0.6393256	-1.6805291	-0.9890554
H	0.2429363	-1.7471290	0.8859903

9. Cartesian coordinates of $[(CH_4)_3(NH_3)]_2$.

$R(Au^{III}\cdots Au^{III})$ = 3.48 Å

C	-1.1588184	-1.7923377	-1.9090000
C	-2.0978184	-2.0123377	0.8770000
C	0.5291816	-1.8473377	1.9030000
C	-0.5470000	1.7430000	1.9030000
C	2.0800000	1.9080000	0.8770000
C	1.1410000	1.6880000	-1.9090000
N	-1.6540000	1.3970000	-0.8760000
N	1.6361817	-1.5013377	-0.8760000
H	-0.7110000	2.7890000	2.1840000
H	-0.1268183	-1.3933377	2.6470000
H	-1.5080000	1.2200000	1.9390000
H	0.6931817	-2.8933377	2.1840000
H	0.1090000	1.2890000	2.6470000
H	1.4901817	-1.3243377	1.9390000
H	-2.3980000	1.7140000	-0.2610000
H	1.7301816	-1.9713377	-1.7730000
H	-1.7480000	1.8670000	-1.7730000
H	2.3801816	-1.8183377	-0.2610000
H	-0.6458184	-1.1233377	-2.6100000
H	2.2100000	1.4530000	-1.9330000
H	0.6280000	1.0190000	-2.6100000
H	-1.0658183	-2.8113377	-2.3010000
H	-2.2278184	-1.5573377	-1.9330000
H	1.0480000	2.7070000	-2.3010000
H	-2.3918183	-1.0613377	1.3270000
H	2.8260000	2.2230000	0.1470000
H	-2.8438183	-2.3273377	0.1470000
H	1.9960000	2.6530000	1.6680000
H	2.3740000	0.9570000	1.3270000
H	-2.0138183	-2.7573377	1.6680000
H	-1.7710000	0.3940000	-1.0320000
H	1.7531816	-0.4983377	-1.0320000
H	0.6243078	1.5719932	-0.9888459
H	1.1557764	1.8223395	0.3912549
H	-0.2571825	1.6441677	0.8868701
H	-1.1737004	-1.9263152	0.3912489
H	0.2389573	-1.7485559	0.8869912
H	-0.6425925	-1.6770483	-0.9885311

$R(Au^{III}\cdots Au^{III})$ = 3.59 Å

C	-1.1410000	-1.6880000	-1.9090000
C	-2.0800000	-1.9080000	0.8770000
C	0.5470000	-1.7430000	1.9030000
C	-0.5106644	1.9557679	1.9030000
C	2.1163356	2.1207679	0.8770000
C	1.1773356	1.9007679	-1.9090000
N	-1.6176644	1.6097679	-0.8760000
N	1.6540000	-1.3970000	-0.8760000
H	-0.6746644	3.0017679	2.1840000
H	-0.1090000	-1.2890000	2.6470000
H	-1.4716644	1.4327679	1.9390000
H	0.7110000	-2.7890000	2.1840000
H	0.1453356	1.5017679	2.6470000
H	1.5080000	-1.2200000	1.9390000
H	-2.3616644	1.9267679	-0.2610000
H	1.7480000	-1.8670000	-1.7730000
H	-1.7116644	2.0797679	-1.7730000
H	2.3980000	-1.7140000	-0.2610000
H	-0.6280000	-1.0190000	-2.6100000
H	2.2463356	1.6657679	-1.9330000
H	0.6643356	1.2317679	-2.6100000
H	-1.0480000	-2.7070000	-2.3010000
H	-2.2100000	-1.4530000	-1.9330000
H	1.0843356	2.9197679	-2.3010000
H	-2.3740000	-0.9570000	1.3270000
H	2.8623356	2.4357679	0.1470000
H	-2.8260000	-2.2230000	0.1470000
H	2.0323356	2.8657679	1.6680000
H	2.4103356	1.1697679	1.3270000
H	-1.9960000	-2.6530000	1.6680000
H	-1.7346644	0.6067679	-1.0320000
H	1.7710000	-0.3940000	-1.0320000
H	-0.6257291	-1.5716351	-0.9882094
H	-1.1560068	-1.8230912	0.3909078
H	0.2561666	-1.6451970	0.8871947
H	0.6622451	1.7848053	-0.9880612
H	1.1922011	2.0368932	0.3909979
H	-0.2194934	1.8572929	0.8873642