

Supporting Information

Synthesis, Electrochemical and Theoretical Studies of the Au(I)-Cu(I) Heterometallic Clusters Bearing Ferrocenyl Groups

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Table S1. Crystal data and structure refinement for **3**.

Identification code	3	
Empirical formula	C ₁₇₄ H ₁₅₁ Au ₆ Cu ₂ F ₁₂ Fe ₆ O ₃ P ₈	
Formula weight	4409.69	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R 3	
Unit cell dimensions	a = 24.7994(3) Å b = 24.7994(3) Å c = 46.1400(7) Å	α = 90° β = 90° γ = 120°
Volume	24574.8(6) Å ³	
Z	6	
Density (calculated)	1.788 Mg/m ³	
Absorption coefficient	6.260 mm ⁻¹	
F(000)	12810	
Crystal size	0.12 x 0.09 x 0.09 mm ³	
Theta range for data collection	2.55 to 25.25°	
Index ranges	-29 ≤ h ≤ 29, -28 ≤ k ≤ 29, -55 ≤ l ≤ 55	
Reflections collected	134450	
Independent reflections	9886 [R(int) = 0.0931]	
Completeness to theta = 25.25°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6027 and 0.5229	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9886 / 63 / 650	
Goodness-of-fit on F ²	1.062	
Final R indices [I > 2σ(I)]	R1 = 0.0449, wR2 = 0.0956	
R indices (all data)	R1 = 0.0650, wR2 = 0.1025	
Largest diff. peak and hole	1.411 and -0.846 e.Å ⁻³	

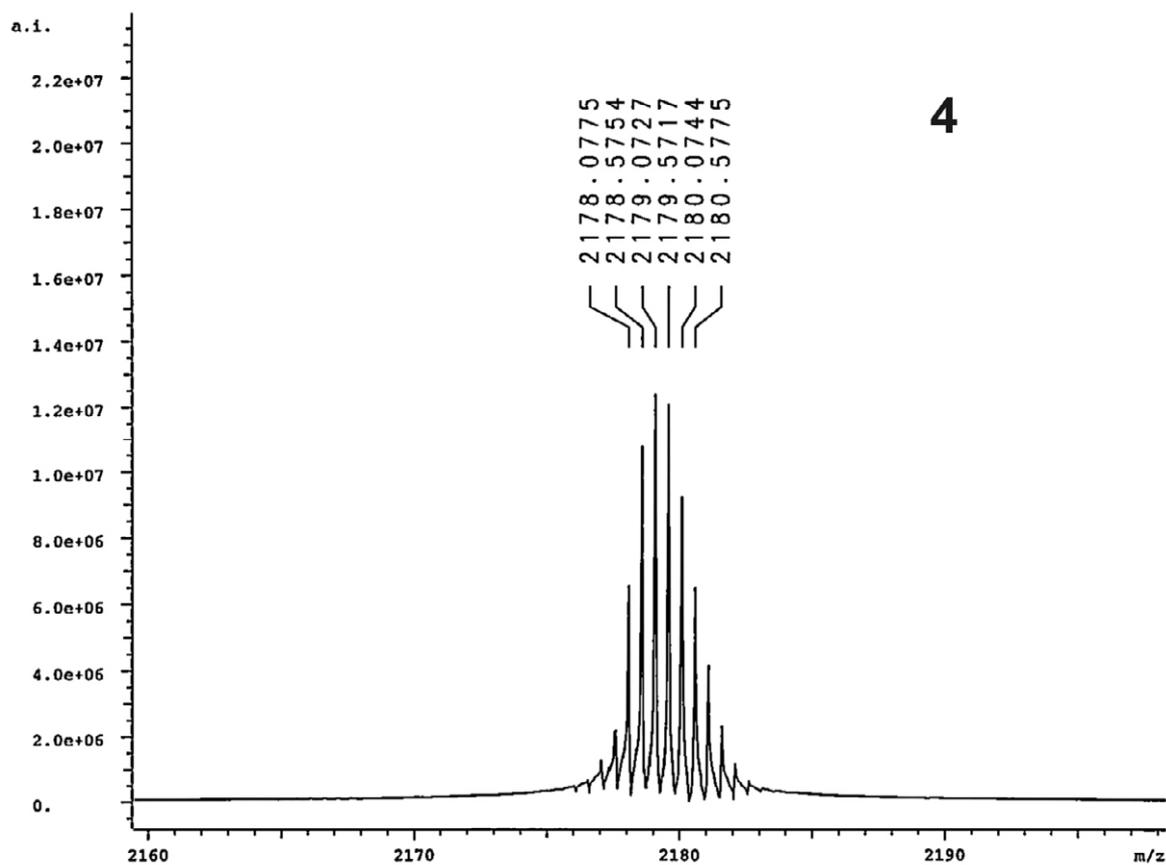
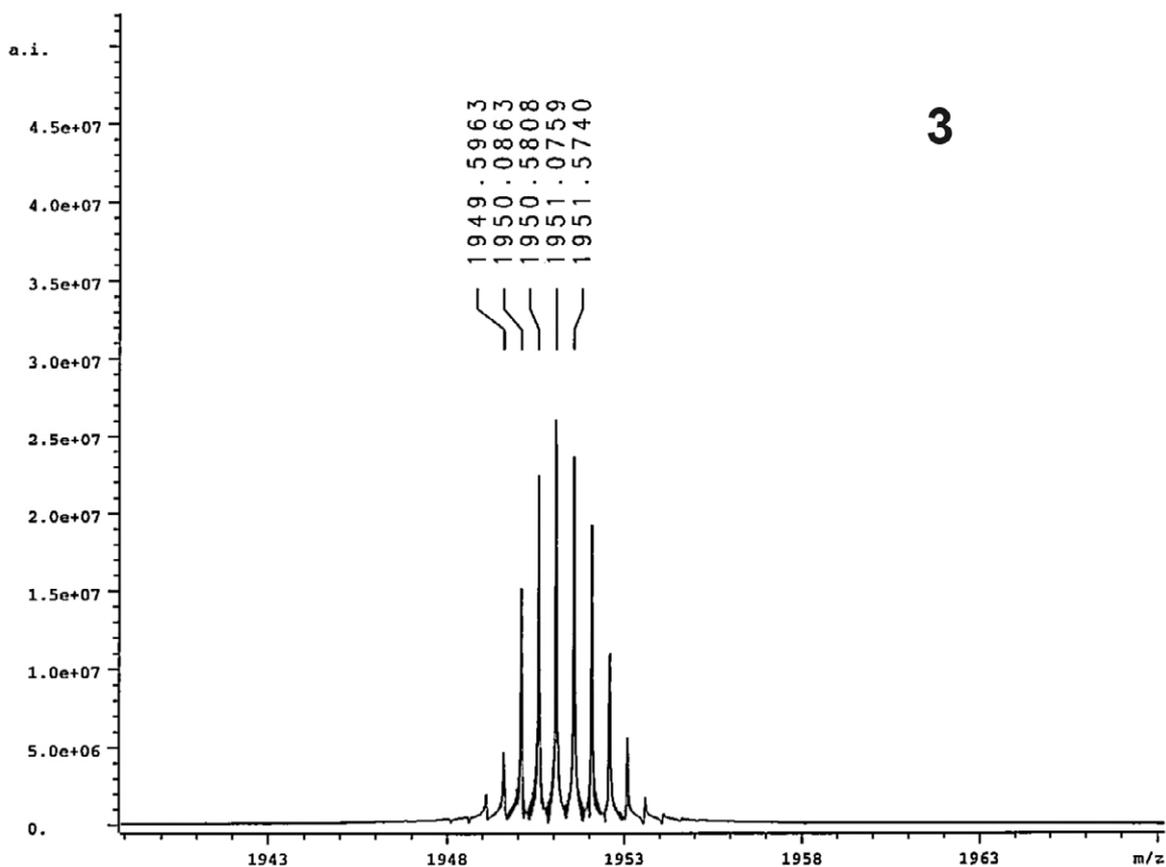


Figure S1. ESI-MS spectra of the $[\{Au_3Cu_2(C_2-R)_6\}Au_3(PPh_2C_6H_4PPh_2)_3]^{2+}$ ($R = Fc$, $R = 4-C_6H_4-Fc$) dications (**3**, **4-2PF₆**).

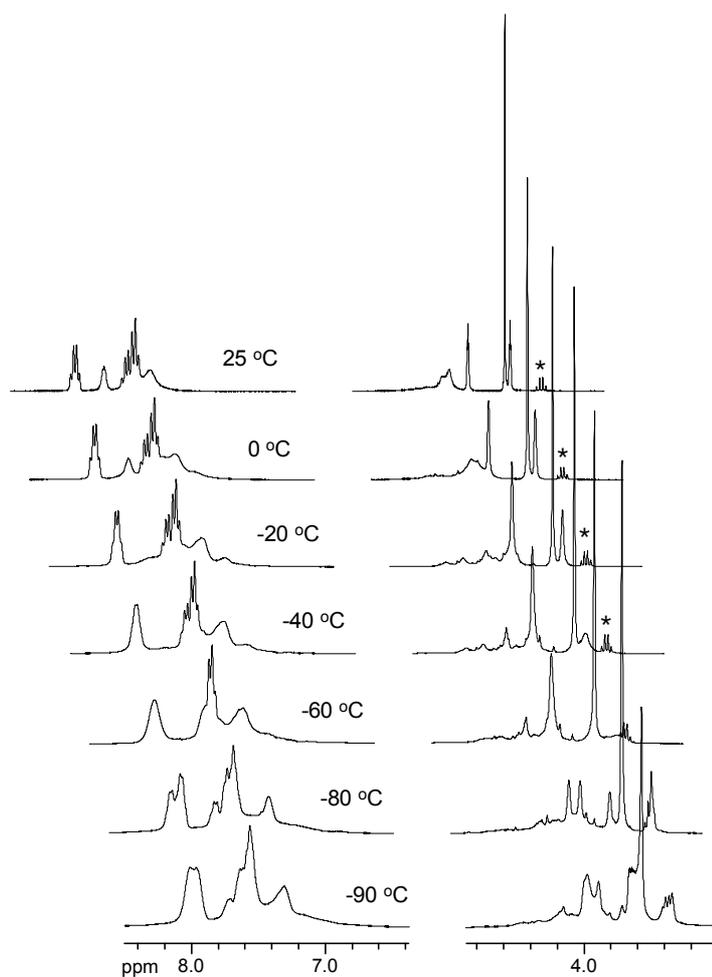


Figure S2. Variable temperature ¹H NMR spectra of **3** (300 MHz, CD₂Cl₂). * denotes admixture.

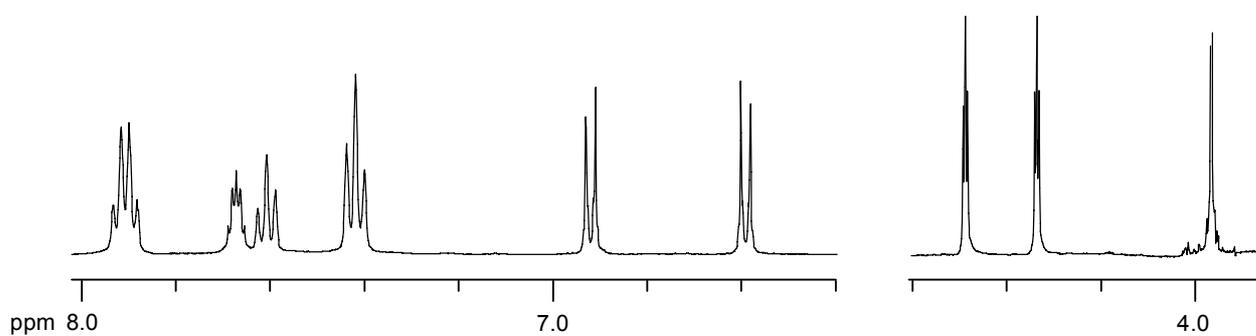


Figure S3. ¹H NMR spectrum of **4** (400 MHz, CD₂Cl₂, 25 °C).

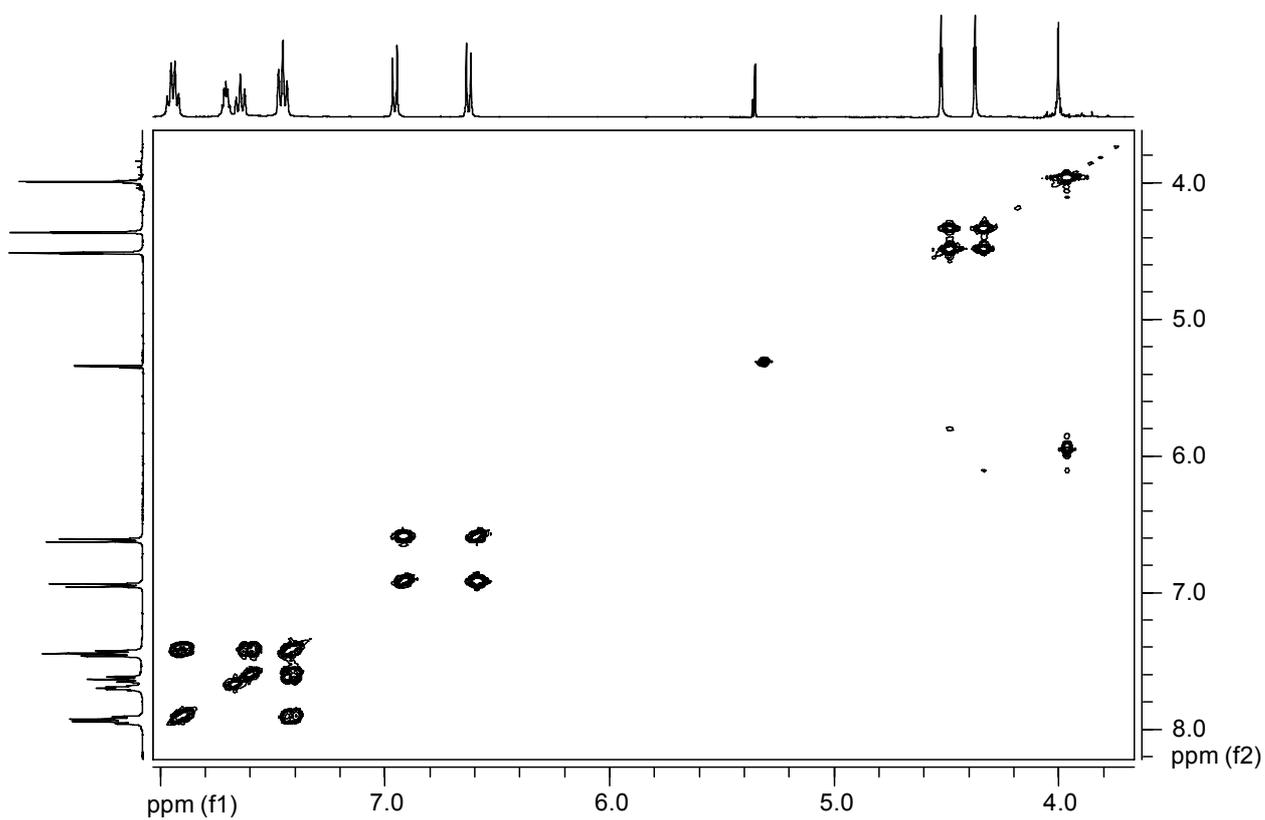


Figure S4. ^1H COSY NMR spectrum of **4** (400 MHz, CD_2Cl_2 , 25°C).

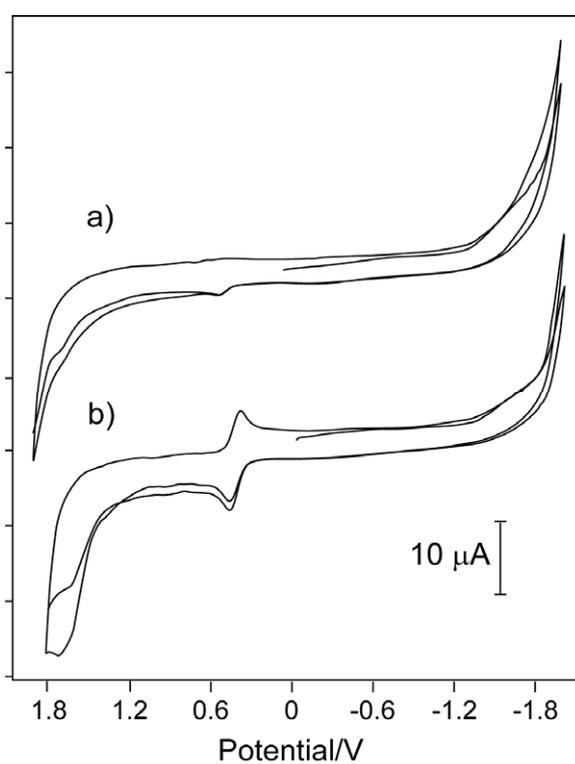


Figure S5. Cyclic voltammograms at GCE of the complexes **1** (a), **2** (b) 0.50 mM in 0.10 M $\text{Bu}_4\text{NPF}_6/\text{CH}_2\text{Cl}_2$ solutions. Potential scan rate 50 mV/s.

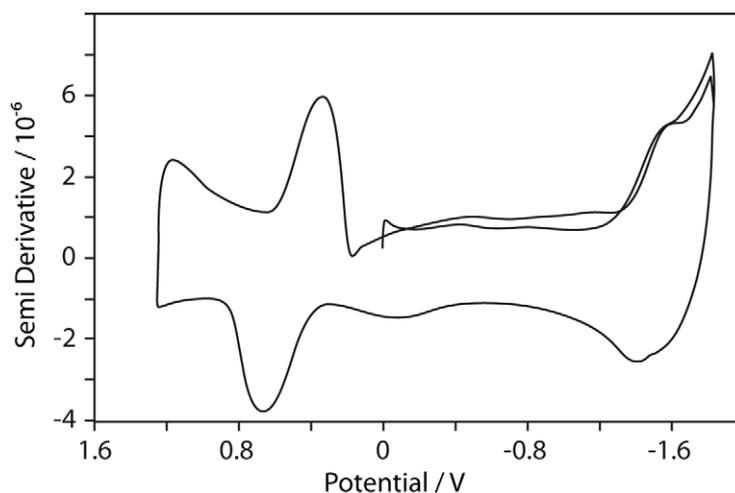


Figure S6. Deconvolution of CV at GCE of **4** (0.40 mM) in 0.10 M solution $\text{Bu}_4\text{NPF}_6/\text{CH}_2\text{Cl}_2$. Temperature 263 K. Potential scan rate 500 mV/s.

Computational supporting information

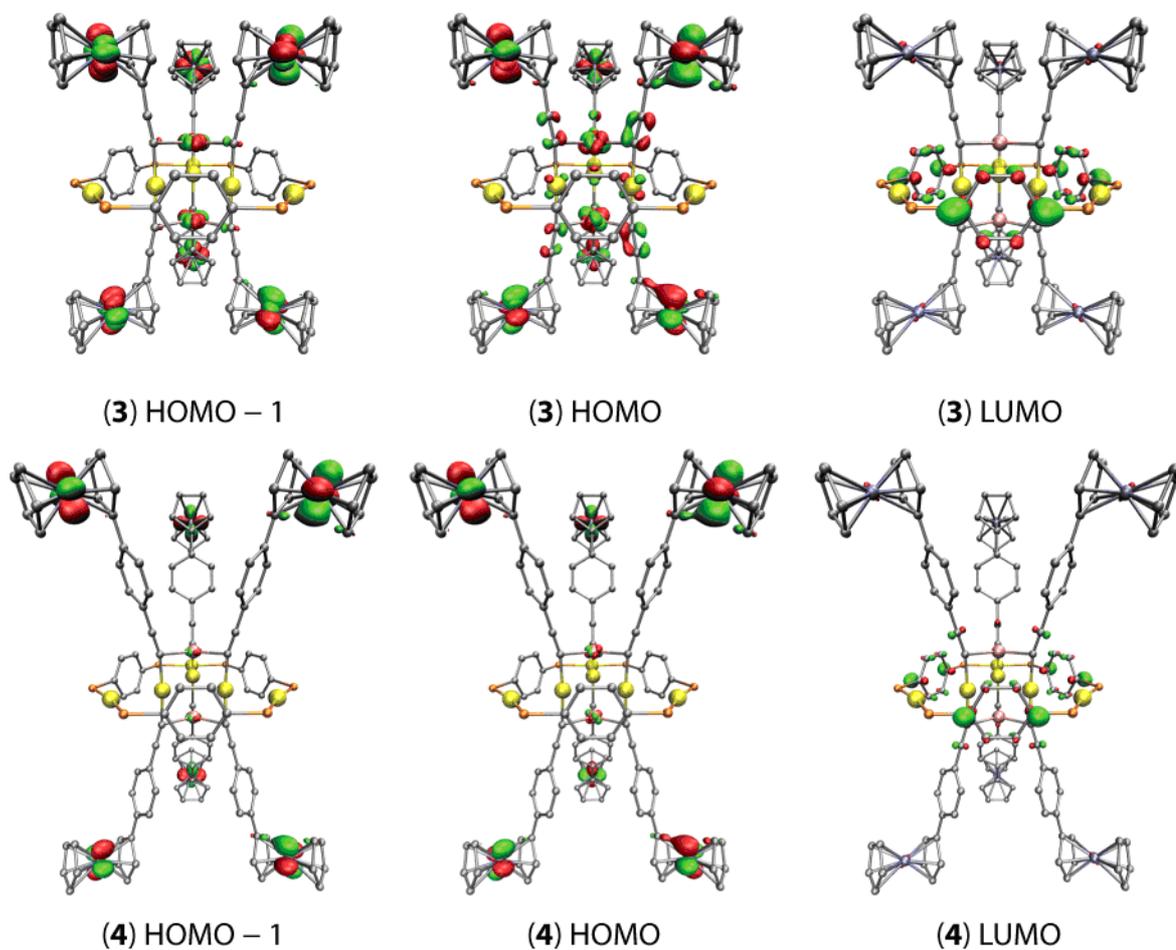


Figure S7. Frontier molecular orbital isodensity plots for the dicationic Au(I)-Cu(I) complexes **3** and **4** in D_{3h} -symmetry (isodensity value 0.04). Phenyl rings of the “belt” fragment and hydrogen atoms omitted for clarity.

Optimized cartesian coordinates of the studied systems in atomic units (BP86 level of theory):

$[\{\text{Au}_3\text{Cu}_2(\text{C}_2\text{Fc})_6\}\text{Au}_3(\text{PPh}_2\text{C}_6\text{H}_4\text{PPh}_2)_3]^{2+}$ (3), C_1 -symmetry

20.77443499411144	16.18313296295928	7.21206098664315	au
17.07016157411250	20.11519405815596	7.30951171993591	au
23.43352956299668	13.52316344661167	11.08081372198537	cu
23.43730475448828	13.52612720803615	3.35340178534569	cu
21.39765044622550	21.52229556243281	-3.29493210898450	fe
15.56626592482316	15.76549029793630	17.83398696310296	fe
13.55136610639898	17.40249128803171	6.56063408259024	p
16.53689884014073	5.49008997816262	8.07678185918591	p
12.39566712557280	17.71512377052582	3.28729870765857	c
14.17933010703894	17.88072722624252	1.30509831409143	c
16.22639457543763	17.88460903595518	1.71750394484169	h
13.34485388168377	18.02526658914518	-1.21218950619200	c
14.74979049548965	18.13353557267966	-2.74504960983970	h
10.74734094209348	18.05611040189972	-1.77029126708713	c
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8.97318865823672	17.93547731113048	0.20152616196070	c
6.93340359573510	17.98124004053741	-0.21876745623315	h
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8.37746906974760	17.66574815118223	4.25018643080865	h
10.81803909113568	18.10302865560271	8.58698716057678	c
10.54356988025904	20.57210749588316	9.56276671143981	c
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8.39951017808118	21.21760601507720	10.98770982099190	c
8.20501927210691	23.14722689108777	11.74658031526212	h
6.52015514780757	19.40198828840331	11.46065115311643	c
4.84366401202042	19.90594424134085	12.58940093657302	h
6.78633923817104	16.93692211239189	10.50396383812134	c
5.31522744632486	15.50890337562312	10.87399041896795	h
8.92258123853254	16.28243013025105	9.07001821092445	c
9.11018606531305	14.34665809705201	8.32425862300286	h
14.19132356777480	13.98104114479587	6.97542914724855	c
14.30338724892616	12.92605377621319	9.42214007208334	c
13.92650072559156	14.09247363188243	11.10462901533764	h
15.40330781413328	9.87251065634995	5.22158961849327	c
15.87336871070045	8.73109558974719	3.54535820218399	h
15.49614271124552	8.81219679688088	7.66809317845155	c
14.91572454122482	10.36525700123050	9.75498578438122	c
14.95374209905161	9.58201760597038	11.68101212939889	h
14.73181521523932	12.41642427499555	4.88491417534866	c
14.65827650671362	13.18891773304910	2.95575007237599	h
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11.22771402203883	6.19429639777726	6.24646722574248	h
10.34498027881393	2.81915314321111	4.07753745379274	c
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13.86399882626116	3.18626183855167	18.38219174747704	h
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23.75143994944724	2.45605782751801	13.82124492922413	h
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24.27342811121152	2.58496075288815	22.15114310854837	h
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28.75552370616986	2.39435368221289	15.11319958818357	h
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16.26044105723218	12.38813885054137	-0.88449442184334	h
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19.68595206045103	9.92990542178068	-5.70567258912214	c
20.13311526988276	9.48420600670413	-7.68359322687945	h
21.14595588143836	9.19301038323260	-3.54471707087547	c
22.94862446747397	8.16861384745017	-3.56796469997946	h
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17.22785287641135	4.36563417996334	0.84634893968183	h
14.35445267218117	6.19128081676299	-1.75439354651838	c
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14.17825791699535	6.23592785816757	-4.46821145888213	c
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16.26761669874146	4.81399751246240	-5.46977423789930	c
16.68015469251172	4.50701752980389	-7.48169317400908	h
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19.44401845360334	2.72153280104454	-3.50467024713607	h
27.06967215232049	14.50090449869981	7.22073368311774	au
32.32758001975139	15.73762685866214	7.28756752229407	au
31.36269355605285	11.31772432789552	-3.30657074651545	fe
29.28775135378927	19.21921139560765	17.85268988007392	fe
31.73574569836588	20.14194816824694	6.54601558377304	p
19.92715038527289	23.51059241349649	8.07187755949601	p
32.58765344743959	20.99570544970135	3.27626059112060	c
31.82965592430646	19.37994785150802	1.28803328613791	c
30.80073813995524	17.60872249557410	1.69420761220449	h
32.37452270964005	20.03706965289643	-1.22687511409649	c
31.75728496947739	18.77581552061702	-2.76432420135632	h
33.71332341264258	22.26518526859181	-1.77695778578580	c
34.15507793792817	22.76049530587645	-3.75170995756661	h
34.50605664330907	23.84951715597561	0.20074954251505	c
35.57601499472814	25.58833833285926	-0.21310400507068	h
33.94069296691860	23.22729893346063	2.71927617458242	c
34.57447104165355	24.48502049188220	4.25186005243305	h
33.70374280351538	22.15431279727807	8.58225477973782	c
35.97415112559602	21.15531625429112	9.56782548559926	c
36.45947006746667	19.15710565866691	9.21494914175212	h
37.59839298402022	22.68702735762664	11.00319515337569	c
39.36262799367023	21.88912785556639	11.76994617833025	h
36.96381529559699	25.22181473174189	11.47683326488963	c
38.23355091025815	26.41996087970178	12.61301664111093	h
34.70049436058903	26.22564554663087	10.51110478108223	c
34.19736096413027	28.21286077128321	10.88270285958134	h
33.07269195628667	24.70549610897842	9.06638661313862	c
31.30617550610755	25.51180294260589	8.31312832704739	h
28.45201484820619	21.29630568013080	6.96243295013246	c
27.47768141482889	21.70277391940252	9.41158485402197	c
28.67272591479871	21.42783651700940	11.09369205478053	h
24.29249127159388	22.32271214550423	5.21084384433521	c
23.07238240178091	22.50444422427213	3.53383684874920	h
23.32350697111271	22.74908623261927	7.65983267594886	c
24.95383417009973	22.45125090336800	9.74725354386697	c
24.25292031784905	22.78832356092930	11.67562720994628	h
26.83146516235228	21.63359028035882	4.87203964816411	c
27.54124850369445	21.33157258850551	2.94091005367407	h
19.34144258421050	26.27209141145205	6.04719951182774	c
21.26306092091523	28.05045322097098	5.51715189935056	c
23.19726627894664	27.74895216366816	6.22857796181465	h
20.71051869402648	30.21315156887616	4.07977400942670	c
22.21710167504876	31.59249011097112	3.67006407323569	h
18.24782293914237	30.62122519917989	3.16836823982012	c
17.82384246065564	32.31762569112945	2.03650261931486	h

16.33153786107841	28.85763194711917	3.68942151012068	c
14.40280906108689	29.16366471854625	2.96582921517747	h
16.87461065862835	26.68658951927313	5.11597671231547	c
15.37691173092847	25.28667955095482	5.50305437222978	h
19.65173310559074	24.67175479863896	11.34389353189874	c
19.60230948936925	27.27985819069492	11.90528566299725	c
19.66718243935431	28.68738799905534	10.37307078051677	h
19.45598466648039	28.09633509955829	14.42793174487166	c
19.40295752281967	30.13614058430270	14.84719462411013	h
19.38207571999748	26.32353333727697	16.40306997300797	c
19.27704467568205	26.96948461356381	18.38098376113702	h
19.42361923290616	23.72489697190295	15.84794431470252	c
19.35939708324341	22.32185216596514	17.38509815886103	h
19.52934522359294	22.88824456627989	13.32987730522317	c
19.53058258420376	20.84092098057198	12.91775213244350	h
26.90484738190170	15.37443277370147	10.94447059804206	c
26.94530009664065	16.13675069621489	13.19093428138117	c
26.81357016146823	17.02056333690587	15.73042278341304	c
25.65461985875232	19.36961627870006	16.58172457740477	c
24.81671952188089	20.80568530466719	15.34391616553855	h
25.71765543333441	19.42649055155574	19.29502627151441	c
24.99226265811749	20.95494647514753	20.49986572320832	h
26.95359330078444	17.16365689471879	20.15912539857169	c
27.32407191636320	16.65728900905756	22.13827812902779	h
27.65731376303662	15.69989169233005	17.98963483592072	c
28.57251347231993	13.83897022118528	18.00381329386476	h
32.43056053565699	20.09232504484388	15.72761207027215	c
32.80213997867883	19.45746528924455	13.78553127783707	h
33.15417691962381	18.78444823750288	17.99610161333044	c
34.20685046015128	16.99934682297342	18.08813422602678	h
32.27397338815759	20.23471379916831	20.12052002005501	c
32.50946280428857	19.73743525290352	22.12293676371607	h
31.00653050398441	22.44077150050779	19.16319939986730	c
30.10299454648144	23.91975307211146	20.30725968730388	h
31.10183494947002	22.35250246736055	16.44659576480701	c
30.30303320636465	23.76959839441955	15.15654481643281	h
27.36501129502918	13.66263280037777	3.49729279058381	c
27.77380461107742	13.01331488385043	1.25192967456392	c
28.10665429993061	12.16716383962027	-1.28177323486676	c
28.15318132898307	9.54622918126497	-2.12884540366288	c
28.02272424991154	7.88683822050213	-0.89222884570809	h
28.31154405104905	9.52090144034926	-4.83813858182317	c
28.38561670255882	7.82816012177429	-6.03932961683302	h
28.41998072848753	12.09615745741848	-5.70340513757755	c
28.57721082542202	12.71174415421361	-7.68007297853401	h
28.32651188288940	13.72319338959707	-3.53810921346618	c
28.30656335008836	15.79657913204769	-3.55604712242681	h
34.49272875815220	11.98594132841381	-1.09093730506126	c
34.47643409338942	12.75454435920491	0.83836541414364	h
34.33926533313858	9.35730406511111	-1.76785827472332	c
34.21168684992875	7.75787315643171	-0.45042905416682	h
34.38302744314798	9.18724725233791	-4.48207553351898	c
34.27356579183214	7.44028180345531	-5.59952320481882	h
34.56024737403257	11.70995989312942	-5.47967473043275	c
34.61371382758365	12.22458397993272	-7.49070228385304	h
34.62942649635607	13.43861411504226	-3.38256398647807	c
34.77681786460393	15.50416647681620	-3.50784015188189	h

$[\{\text{Au}_3\text{Cu}_2(\text{C}_2\text{Fc})_6\}\text{Au}_3(\text{PPh}_2\text{C}_6\text{H}_4\text{PPh}_2)_3]^{2+}$ (3), D_{3h} -symmetry

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-1.91866807456961	3.32323058801486	0.00000000000000	au
3.83733614913923	0.00000000000000	0.00000000000000	au

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-4.66740943497781	8.08419028110789	0.000000000000000	au
9.33481886995564	0.000000000000000	0.000000000000000	au
0.000000000000000	0.000000000000000	3.69606127309077	cu
0.000000000000000	0.000000000000000	-3.69606127309077	cu
-0.96626717815601	-10.66439244328063	0.000000000000000	p
-8.75250118272979	-6.16900814476651	0.000000000000000	p
-0.96626717815601	10.66439244328063	0.000000000000000	p
-8.75250118272979	6.16900814476651	0.000000000000000	p
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9.71876836088580	4.49538429851412	0.000000000000000	p
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-1.97843125989019	3.42674346141230	3.82718976643638	c
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-1.97843125989019	-3.42674346141230	-3.82718976643638	c
3.95686251978038	0.000000000000000	-3.82718976643638	c
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5.43337495009705	-6.75813098842681	2.29632977920666	c
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-8.56940059312889	-1.32637524085668	-2.29632977920666	c
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13.48650594229237	-4.28567294969650	3.72663921713409	c
11.28730253556140	-8.32329576034589	3.47377310221487	c
15.14453526653634	-5.29933052415919	5.53530133739852	c
12.93617359528976	-9.32406194804470	5.29605389581579	c
14.87097116022848	-7.81912891752649	6.32404435533695	c
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15.14453526653634	5.29933052415919	5.53530133739852	c
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14.87097116022848	-7.81912891752649	-6.32404435533695	c
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-11.88294982669731	12.36595523690273	6.33966496874439	h
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-5.48942933658282	9.50797051552048	-6.46598291882716	h

[{Au₃Cu₂(C₂C₆H₄Fe)₆}Au₃(PPh₂C₆H₄PPh₂)₃]²⁺ (4), C₁-symmetry

-2.41595586048594	2.98969180007775	-0.26053809124009	au
-5.84737518391877	7.19612876018849	0.22723142601349	au
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0.01728032808449	0.05895712475037	-3.89569657518239	cu
-4.93054647642222	9.26132245702055	-18.69929165919989	fe
-9.79378694084884	3.13239352049285	18.00894478237846	fe
-9.55154537736194	4.68527165789457	-0.18419965377063	p
-7.24729048694013	-7.40194502638278	0.94154465856464	p
-10.96468109790055	5.15814793578112	-3.33304604523760	c
-9.32993581283531	5.38106886862380	-5.43550777354729	c
-7.26130428895571	5.27553141407839	-5.18042900207133	h

-10.33485525197753	5.72437972158962	-7.86903700447257	c
-9.04119895214155	5.87798804906740	-9.49454662082982	h
-12.96367656112214	5.88327542496505	-8.21812687676968	c
-13.74910256338385	6.17342803729317	-10.12587494631078	h
-14.59142272497383	5.69005912538266	-6.12798014330610	c
-16.65332568004499	5.83378140288762	-6.38920353767353	h
-13.60338635757140	5.32212989696476	-3.69104993504400	c
-14.89993793505359	5.18707928936404	-2.06799201763140	h
-12.01240046158768	5.49311447150676	2.13222207841509	c
-11.95646310738929	7.89904347877977	3.28726579704992	c
-10.38877931177530	9.20923432013339	2.86435929154298	h
-13.87894362344616	8.62029948405850	4.97047186214056	c
-13.81924770104103	10.50289546413878	5.85967650996544	h
-15.86326065817929	6.94347284807944	5.52254517761424	c
-17.37011136008316	7.50910395052870	6.84531630269821	h
-15.92267694046459	4.53934530152010	4.39092163867448	c
-17.47383248553099	3.21798752370949	4.82443406161159	h
-14.00993926530856	3.81068594143368	2.70102747718787	c
-14.07261434642452	1.91996789183207	1.82922706347329	h
-9.05672336989995	1.23548272584792	0.13848749434711	c
-8.90034362911606	0.12226876255541	2.55861117608592	c
-9.16477990748286	1.27188042869822	4.27358955763267	h
-8.13449408972302	-2.87826523940710	-1.74198210453341	c
-7.79783439038966	-4.01786429058597	-3.45019927719508	h
-8.03389227348029	-4.00424681287339	0.67494013329519	c
-8.41444668845569	-2.47395366430858	2.82373491677783	c
-8.32566989352532	-3.29538692407832	4.73384445147567	h
-8.65923790283570	-0.29389489716296	-2.01017169096498	c
-8.74030993910388	0.52445876210404	-3.92124157361568	h
-9.32886340601589	-8.99676435115188	-1.33966899939103	c
-11.78402159591343	-8.08408011321721	-1.87001379149168	c
-12.46429513935442	-6.32416624328828	-0.98778919792599	h
-13.36591366363830	-9.41472229207979	-3.53529746790213	c
-15.27761358018876	-8.69221324884488	-3.94003379366255	h
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-13.76615826724541	-12.69802507746157	-5.98459794494678	h
-10.07616770410183	-12.56823184987362	-4.16710332879815	c
-9.39782902562558	-14.31792455650656	-5.07068062527216	h
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-6.55701044332019	-11.94453058148252	-2.12290237167271	h
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-10.72331852907798	-9.45382784463748	4.51699602762627	c
-12.03761955594094	-9.73355076588018	2.92696901733510	h
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-13.33169440941856	-11.03013902801318	7.26632063501290	h
-9.78421133462455	-9.86971254342545	9.00664259275986	c
-10.36126618267996	-10.45630595499821	10.92071631957683	h
-7.37819271803737	-8.81732421724259	8.60356438356936	c
-6.05390068358675	-8.56631005631332	10.19184391382236	h
-6.63155372252512	-8.08980001419828	6.16179955566569	c
-4.73219113662391	-7.27956687566190	5.85846399212690	h
-2.88369366813673	2.95998168024308	3.53296947340689	c
-3.50108064193040	3.19543295280524	5.81026817785947	c
-6.89934165005821	4.86222569259144	16.04655360815236	c
-5.96757352930653	3.64334068869942	18.31683586427071	c
-4.54531291846917	2.13342376160391	18.39153979564603	h
-7.24144159073058	4.71484064216217	20.46086146528259	c
-6.95568698307237	4.17150051043216	22.44426555467962	h
-8.98540982000347	6.59063202234946	19.55269252430120	c
-10.25989949766755	7.74275375837281	20.71871453437022	h
-8.80194682205224	6.67037228177221	16.84554313512784	c
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-14.32363073021386	3.57608781507577	15.15205123803771	h
-13.41099515782828	2.30352546165196	19.13773244238056	c
-14.63157379164567	3.51430418406741	20.30226512951916	h
-11.67142583196585	0.42910417619916	20.06265133971651	c
-11.33138791599684	-0.03918895228089	22.05690270007420	h
-10.42828939502960	-0.69499938037958	17.91931399548915	c
-8.97467233662062	-2.17609733330060	17.99338649450264	h
-2.20437970871271	3.28823647909596	-4.06422977153725	c
-2.35014033948466	3.89827720800944	-6.34978547244734	c
-2.66852816155345	6.63639489396891	-16.91027338486921	c
-1.17756413520213	8.59094853608191	-18.13257464052898	c
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-1.74062364990728	8.57508527842800	-20.78755034545335	c
-0.91383315772985	9.83863259879451	-22.21262977916546	h
-3.60521408902539	6.65186242150537	-21.24217680827521	c
-4.46220615085003	6.18897680458592	-23.07570147975216	h
-4.19195567567457	5.47062470801959	-18.87068125960354	c
-5.57657971017436	3.94833938678915	-18.60281101184368	h
-7.24046519589004	10.87030241511164	-16.02114167532121	c
-7.23616791808711	10.40065578998874	-13.99738960088737	h
-5.70440207949491	12.76655979876320	-17.21984841996907	c
-4.34920632739315	14.02297128867959	-16.27251640145206	h
-6.23916705027142	12.71593005875590	-19.88685842913941	c
-5.36088410499949	13.92057730191231	-21.33243941203609	h
-8.10228332656352	10.78656923296280	-20.33371299422877	c
-8.89314607462926	10.26029333334771	-22.18025834669378	h
-8.71963396430391	9.64282154355258	-17.94385954157271	c
-10.06899228708583	8.09214718415896	-17.64832103520545	h
-1.08664363703898	-3.32069862305325	0.12498059111622	au
-2.92115522630220	-8.43833869249327	0.34969445036663	au
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4.51003536187890	-15.96732161618780	4.10943610948069	c
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4.10738134102043	-8.65699214104122	4.12868796138397	h
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7.42746516502477	-4.24192123890447	-3.54875538536252	h
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-0.45684645611249	9.26605107499702	-13.01114043565243	h

[{Au₃Cu₂(C₂C₆H₄Fc)₆}Au₃(PPh₂C₆H₄PPh₂)₃]²⁺ (4), D_{3h}-symmetry

-1.87308074513357	-3.24427101725038	0.00000000000000	au
-1.87308074513357	3.24427101725038	0.00000000000000	au
3.74616149026731	0.00000000000000	0.00000000000000	au
-4.61966278439853	-8.00149065641336	0.00000000000000	au
-4.61966278439853	8.00149065641336	0.00000000000000	au
9.23932556879703	0.00000000000000	0.00000000000000	au
0.00000000000000	0.00000000000000	3.71022778218611	cu
0.00000000000000	0.00000000000000	-3.71022778218611	cu
-0.97035602442828	-10.63829218785759	0.00000000000000	p
-8.72785327535203	-6.15949906179891	0.00000000000000	p
-0.97035602442828	10.63829218785759	0.00000000000000	p
-8.72785327535203	6.15949906179891	0.00000000000000	p
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9.69820929978025	4.47879312605862	0.00000000000000	p
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-1.96037092450592	3.39546204292502	3.82412197398702	c
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