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Supporting Information

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Structure and Bonding in Neutral and Cationic 14-Electron Gold-Alkyne π-Complexes

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Crystal Structure Determinations by X-ray Analysis

Definitions:

$R_{int} = \Sigma \mid F_o^2 - F_o^2(\text{mean}) \mid / \Sigma [F_o^2]$

$R_1 = \Sigma \mid |F_o| - |F_c| \mid / \Sigma |F_o|$

$wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{½}$

X-ray Crystal Structure Analysis of Cyclododecyne (5): $C_{12}H_{20}$, M_r = 164.28 g · mol^{-1}, colorless cylinder, crystal size 0.50 x 0.40 x 0.40 mm, monoclinic, space group $P2_1/c$, a = 9.1005(7) Å, b = 13.5069(11) Å, c = 16.9276(14) Å, β = 90.073(4)°, V = 2080.7(3) Å^3, T = 100 K, Z = 8, D_{calc} = 1.049 g·cm^3, λ = 1.54178 Å, $\mu(Cu\text{-}K_\alpha)$ = 0.420 mm^{-1}, empirical absorption correction (T_{min} = 0.18, T_{max} = 0.86), Proteum X8 diffractometer, 4.19 < θ < 68.11°, 36475 measured reflections, 3664 independent reflections, 2927 reflections with $I > 2\sigma(I)$, Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.076 [$I > 2\sigma(I)$], wR_2 = 0.175, 214 parameters, H atoms riding, S = 1.158, residual electron density +0.3 / -0.3 e Å^{-3}.

The crystal was grown from the melt by cooling to 100 K, heating to 220 K (–53 °C) in a 0.5 mm diameter capillary. Before the crystallization experiment on the diffractometer, a DSC analysis was undertaken in order to determine the thermal properties in the range 25 to –100 ºC. We observed a small exothermic transition on the melting curve that may be due to the formation of a stable phase containing rotating molecules (Figure S-1). The packing diagram at –173 ºC shows that the molecules pack as discs that stack along the c axis (Figure S-2). At 220 K the unit cell is a = 9.1590(6), b = 13.6238(9), c = 17.130(1) Å and β = 88.912 deg (volume of the unit cell at 220 K is 2137.1(2) Å^3). The two independent molecules in the asymmetric unit are approximately related by a non-crystallographic center of symmetry. The two molecules adopt very similar conformations despite very different crystal environments (Figure S-3 and S-4). CCDC 715728.

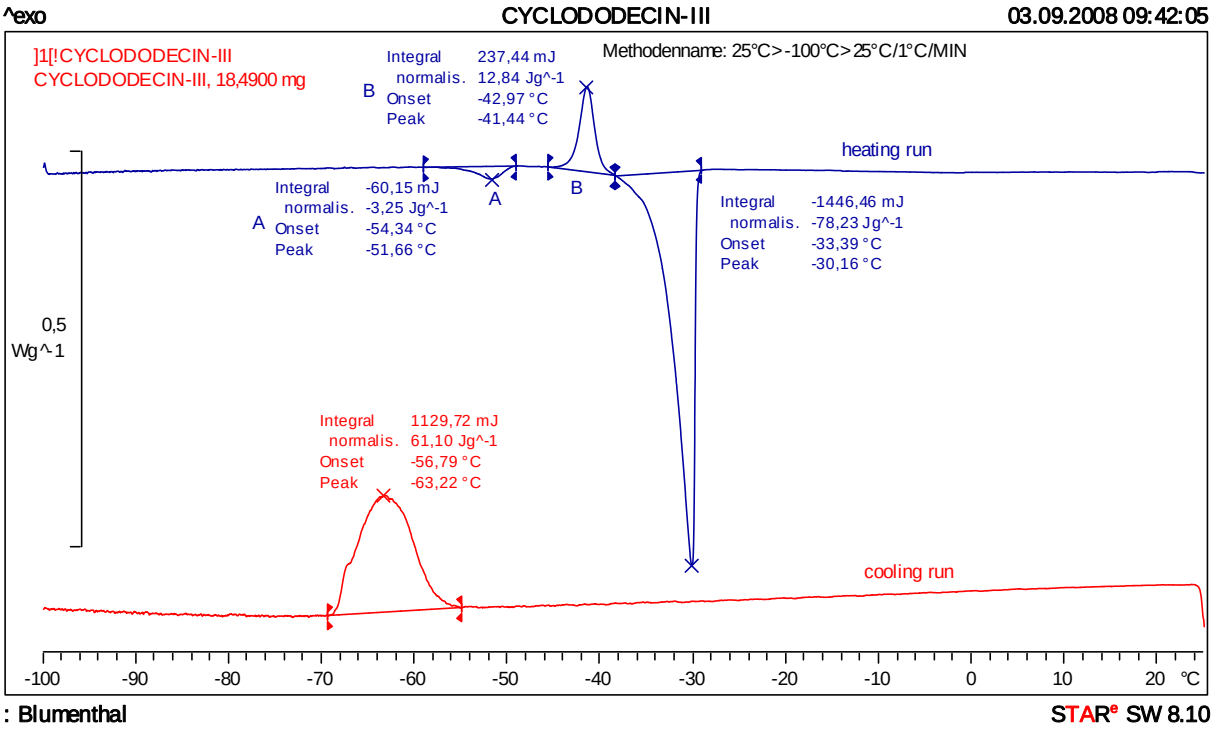

Figure S-1. DSC cooling and heating curves for cyclododecyne (Mettler-Toledo TA820 microcalorimeter, STAR software, 18.49 mg cyclododecyne, 25 > T > –100 ºC, scan rate 1 ºC/min, ordinate: heat flow).

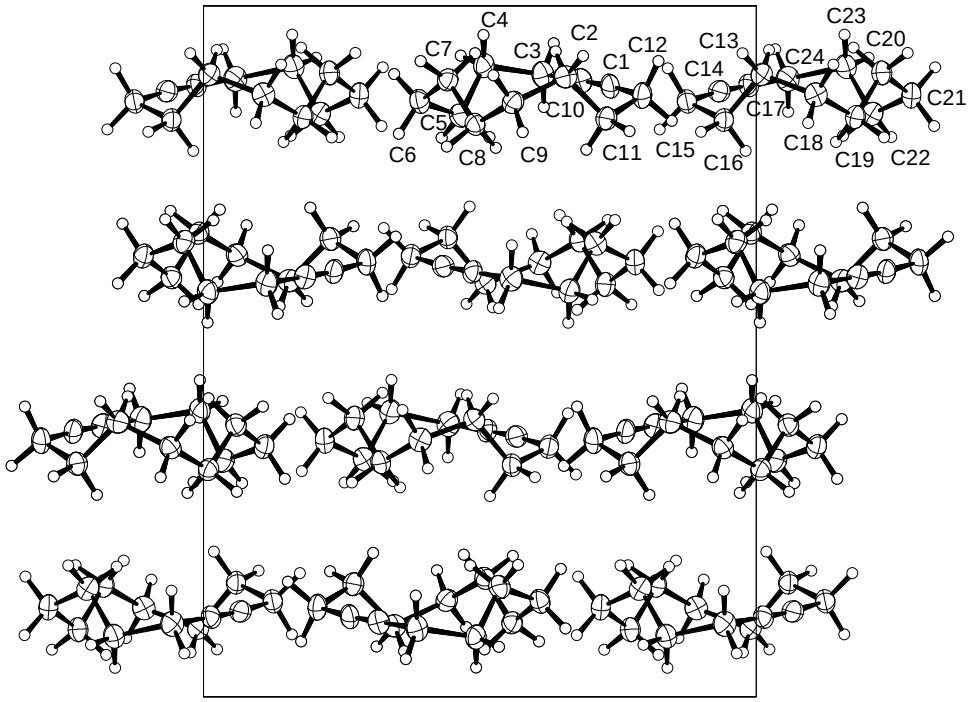

Figure S-2. The unit cell of solid cyclododecyne (**5**), viewed down *a* looking towards the origin showing the sheet structure of the molecules.

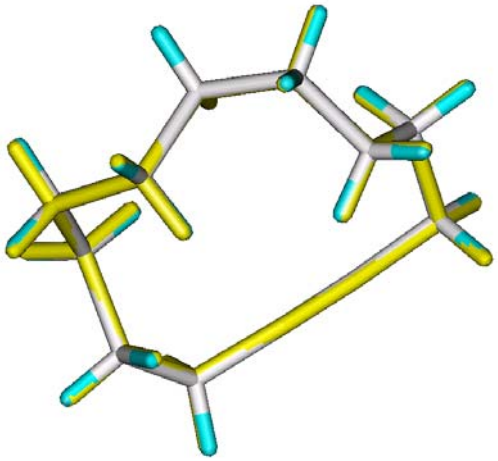

Figure S-3. Superposition of the two independent molecules in the crystal structure of cyclododecyne (**5**), showing the conformational similarity despite different crystal environments.

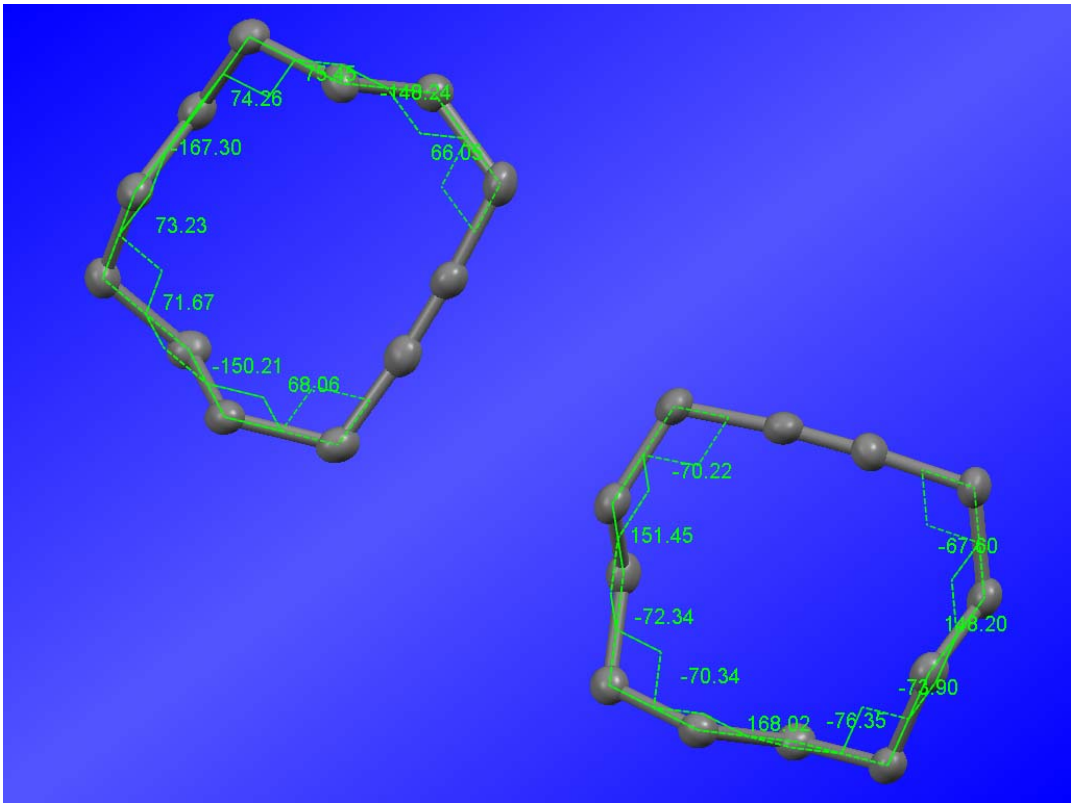

Figure S-4. Torsion angles of the two independent molecules of cyclododecyne (**5**) in the solid state; note that the compound adopts a planar chiral conformation and the crystal is a racemate.

X-ray Crystal Structure Analysis of 6: $C_{12}H_{20}AuCl$, M_r = 396.70 g · mol^{-1}, colorless prism, crystal size 0.13 x 0.04 x 0.02 mm, monoclinic, space group *C2/c*, *a* = 54.7070(11) Å, *b* = 11.7361(2) Å, *c* = 15.6081(3) Å, β = 97.166(1)°, *V* = 9942.9(3) Å^3, *T* = 100 K, *Z* = 32, D_{calc} = 2.120 g·cm^3, λ = 0.71073 Å, μ(*Mo-K*$_\alpha$) = 12.014 mm^{-1}, empirical absorption correction (T_{min} = 0.22, T_{max} = 0.74), Nonius KappaCCD diffractometer, 5.10 < θ < 28.28°, 128853 measured reflections, 12273 independent reflections, 9302 reflections with $I > 2\sigma(I)$; structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.026 [$I > 2\sigma(I)$], wR_2 = 0.065, 522 parameters, H atoms riding, *S* = 1.030, residual electron density +1.7 / –1.4 e Å^{-3}.

There are four independent molecules in the asymmetric unit, which associate as dimers with Au···Au distances of around 3.3 Å (Figure 3 and S-5). The angle between the midpoint of the C≡C triple bond, the Au atom and the Cl atom has a mean value of 176(1)°. Figure S-5 shows the superposition of the two independent molecule pairs in the crystal. Several crystals were investigated, and the results described here are from what is judged to be the best crystal (crystals decompose after a few minutes at ambient temperature). The crystal chosen appears to have a slight satellite, which manifests itself as a reflection of the structure across the (1 0 2) plane. It was only possible to locate the contribution from the Au atoms resulting from the satellite, which refined to an occupancy of 0.0407(7), giving a satellite impurity of circa 4 %. CCDC 715727.

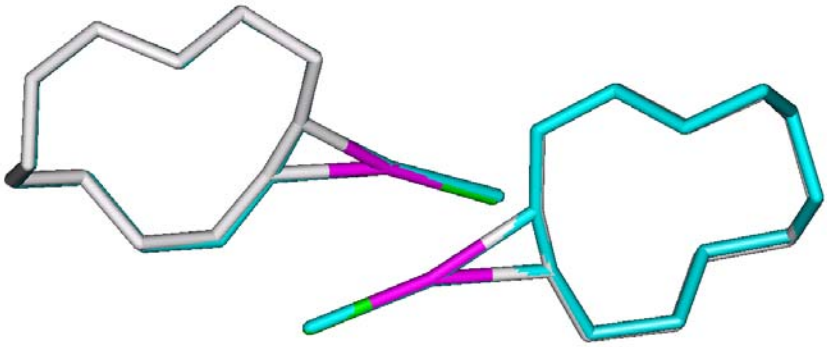

Figure S-5. Superposition of the two independent molecule pairs in the crystal structure of **6**.

X-ray Crystal Structure Analysis of 8: $[C_{39}H_{56}AuN_2]^+[SbF_6]^-$, M_r = 985.57 g · mol^{-1}, colorless plate, crystal size 0.14 x 0.09 x 0.05 mm, orthorhombic, space group *Pna2*$_1$, a = 16.1859(2) Å, b = 14.7429(2) Å, c = 34.0181(4) Å, V = 8117.64(18) Å^3, T = 100 K, Z = 8, D_{calc} = 1.613 g·cm^3, λ = 0.71073 Å, μ(*Mo-K*$_\alpha$) = 4.331 mm^{-1}, empirical absorption correction (T_{min} = 0.51, T_{max} = 0.77), Nonius KappaCCD diffractometer, 5.86 < θ < 33.22°, 164022 measured reflections, 30681 independent reflections, 24434 reflections with $I > 2\sigma(I)$, Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.035 [$I > 2\sigma(I)$], wR_2 = 0.057, 880 parameters, absolute structure parameter = 0.4144(19), H atoms riding, S = 1.020, residual electron density +2.5 / –1.4 e Å^{-3}.

The gold and antimony atoms form an approximately centrosymmetric arrangement in the unit cell and hence do not appreciably contribute to the anomalous signal. The structure was refined as a racemic twin and the twin occupation parameter refined to 0.4144(19) and the unweighted R-index dropped by ca. 0.01. Part of the aliphatic chain in one of the independent cyclododecyne ligands in the unit cell is disordered. As a consequence, some of the bond distances in the chain differ from expected values, expecially at the regions of the transition from disorder to non-disorder. Figure S-6 shows a superposition of the two independent anions and cations in the unit cell. CCDC 715729.

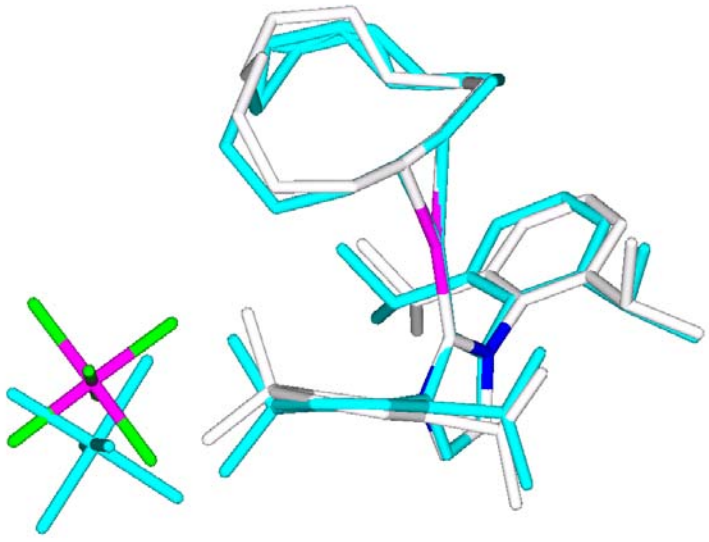

Figure S-6. Superposition of the two independent anions and cations in the crystal structure of **8**.

X-ray Crystal Structure Analysis of 9: $C_{28}H_{40}AuClN_2 \cdot CHCl_3$, M_r = 756.40 g · mol^{-1}, colorless plate, crystal size 0.33 x 0.24 x 0.18 mm, orthorhombic, space group $P2_12_12_1$, a = 10.6707(2) Å, b = 16.5339(4) Å, c = 17.7935(4) Å, V = 3139.28(12) Å^3, T = 100 K, Z = 4, D_{calc} = 1.600 g·cm^3, λ = 0.71073 Å, $\mu(Mo\text{-}K_\alpha)$ = 5.047 mm^{-1}, empirical absorption correction (T_{min} = 0.62, T_{max} = 1.00), Nonius KappaCCD diffractometer, 2.98 < θ < 31.56°, 10398 measured reflections, 10398 independent reflections, 10014 reflections with $I > 2\sigma(I)$, Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.041 [$I > 2\sigma(I)$], wR_2 = 0.127, 333 parameters, absolute structure parameter = 0.178(7), H atoms riding, S = 1.027, residual electron density +2.2 / –1.7 e Å^{-3}. CCDC 715730.

X-ray Crystal Structure Analysis of 10: $[C_{40}H_{60}AuN_2]^+ \cdot 2\,[Ag]^+ \cdot 3\,[SbF_6]^- \cdot [H_2O]$, M_r = 1706.87 g · mol^{-1}, colorless plate, crystal size 0.16 x 0.10 x 0.04 mm, monoclinic, space group $C2/m$, a = 18.1953(3) Å, b = 15.7767(3) Å, c = 19.0602(3) Å, β = 97.675(1)°, V = 5422.44(16) Å^3, T = 100 K, Z = 4, D_{calc} = 2.091 g·cm^3, λ = 0.71073 Å, $\mu(Mo\text{-}K_\alpha)$ = 4.970 mm^{-1}, empirical absorption correction (T_{min} = 0.42, T_{max} = 0.88), Nonius KappaCCD diffractometer, 6.83 < θ < 33.21°, 68408 measured reflections, 10510 independent reflections, 8640 reflections with $I > 2\sigma(I)$, Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.044 [$I > 2\sigma(I)$], wR_2 = 0.130, 313 parameters, H atoms riding, S = 1.045, residual electron density +2.9 / –3.4 e Å^{-3}.

The cyclododecyne ligand is disordered (occupancy C2A-C6A:C2B-C6B 0.5:0.5). Disordered atoms were refined with isotropic atomic displacement parameters. Hydrogen atoms were calculated and refined using a riding model. Distances and angles within the disordered cyclododecyne ligand are poor but it is likely that C6A is not bonded to its [x, -y, z] symmetry related equivalent but that of 6B. Hydrogen atoms for this part of the chain were calculated accordingly. The silver atoms are bridged by what is most likely trace water (Figure S-7). CCDC 715731.

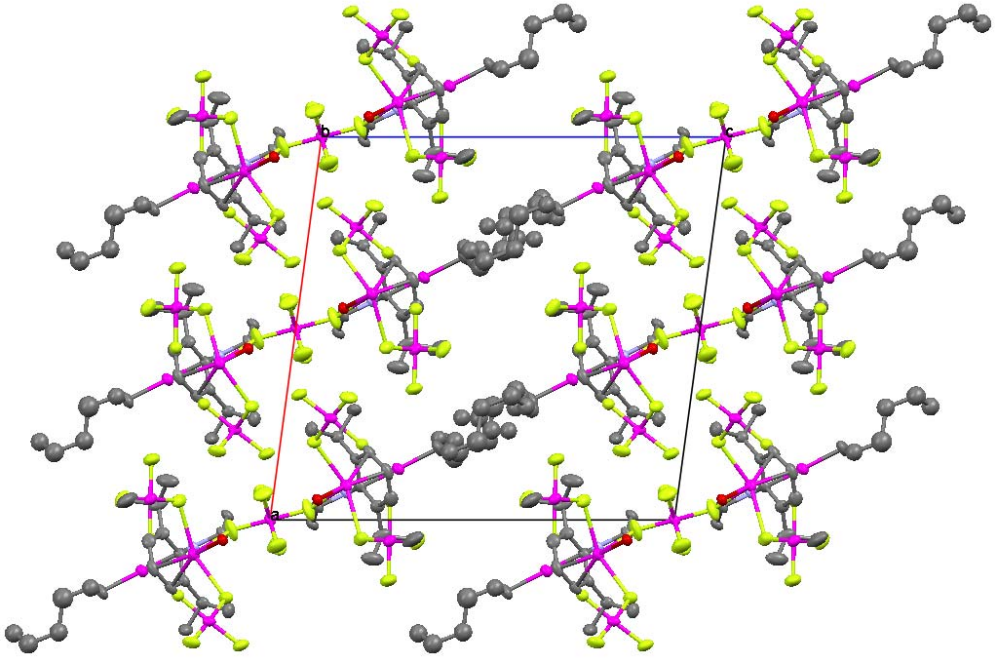

Figure S-7. Packing of the ions and molecules of **10** in the crystal viewed along *b* away from the origin (C: gray; N: blue; O: red; F: lime green; Au, Ag, Sb: magenta).

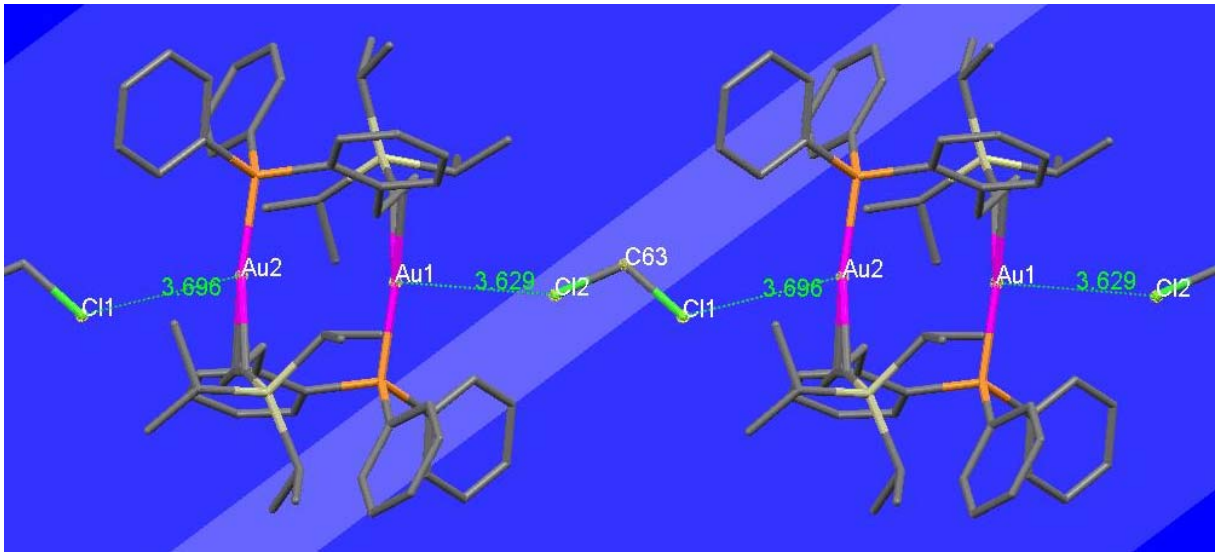

Figure S-8. Structure of complex **1** reported by Shapiro and Toste,[1] where the two independent P–Au–alkyne(midpoint) units are noticeably bent (173°) and the gold atoms point toward solute dichloromethane (mean Au···Cl distance 3.66 Å).

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1 N. D. Shapiro, F. D. Toste, *Proc. Natl. Acad. Sci. USA* **2008**, *105*, 2779-2782.

Computational Studies

Coordinates (Å) and total energies (a.u.) of the structures of cyclododecyne (5) and complexes 6-10 optimized at the BP86(RI)/def2-TZVP level.

Cyclododecyne (**5**)
32
Energy = -469.4407637312

C	0.6123438	2.1423543	-0.0428171
C	-0.6002773	2.1454954	0.0419856
C	-2.0504562	2.0207894	0.1742133
H	-2.5435963	2.3650060	-0.7516734
H	-2.4100246	2.6848328	0.9778150
C	-2.4697418	0.5624851	0.4804390
H	-1.9390456	0.2460369	1.3918153
H	-3.5446102	0.5439991	0.7226210
C	-2.1730634	-0.4141351	-0.6703934
H	-1.2715858	-0.0703419	-1.2030614
H	-2.9939383	-0.3687787	-1.4042352
C	-1.9616228	-1.8700636	-0.2165780
H	-2.7805748	-2.1608479	0.4631581
H	-2.0396759	-2.5403165	-1.0892674
C	-0.6079547	-2.1070204	0.4781952
H	-0.6337898	-3.0673485	1.0189932
H	-0.4638378	-1.3351668	1.2524923
C	0.5961951	-2.1075011	-0.4796668
H	0.4557927	-1.3317048	-1.2506342
H	0.6179279	-3.0656189	-1.0245677
C	1.9504887	-1.8793618	0.2169044
H	2.0233157	-2.5503264	1.0894803
H	2.7686913	-2.1746912	-0.4617639
C	2.1696260	-0.4246859	0.6710629
H	2.9892176	-0.3839766	1.4066237
H	1.2689927	-0.0757028	1.2018317
C	2.4743022	0.5501197	-0.4791805
H	3.5496195	0.5258747	-0.7188589
H	1.9440803	0.2362702	-1.3917522
C	2.0619750	2.0106855	-0.1743576
H	2.5562314	2.3532469	0.7515640
H	2.4251868	2.6723562	-0.9782806

Au(NHC) (**7**)
66
Energy = -1296.203259535

C	1.2449843	0.6038921	3.1165162
C	0.0012180	0.7947818	2.4787990
C	-1.2418059	0.6065519	3.1187584
C	-1.2056748	0.1950741	4.4581005
C	0.0027909	-0.0117132	5.1190566
C	1.2105705	0.1916403	4.4555952
N	0.0003913	1.2379025	1.0934847
C	-0.0002412	0.4358386	0.0000838
N	-0.0010314	1.2378766	-1.0934160

C	-0.0010586	2.5628729	-0.6822912
C	-0.0003626	2.5628676	0.6821899
C	-0.0015013	0.7945370	-2.4785583
C	-1.2450610	0.6022032	-3.1162879
C	-1.2103260	0.1900189	-4.4553858
C	-0.0025323	-0.0130411	-5.1188399
C	1.2057593	0.1936694	-4.4574360
C	1.2415656	0.6053996	-3.1182213
C	-2.5857386	0.8291571	-2.4293701
C	-3.4218046	-0.4629647	-2.3846514
C	2.5826363	0.8373732	-2.4338490
C	3.4298807	-0.4475975	-2.4014037
C	-2.5830545	0.8369722	2.4342619
C	-3.4257090	-0.4510899	2.3966713
C	2.5854342	0.8302461	2.4290602
C	3.4168530	-0.4646429	2.3766710
C	-3.3707793	1.9731872	-3.0991046
C	3.3558161	1.9928279	-3.0980420
C	-3.3608727	1.9872793	3.1016613
C	3.3754535	1.9677432	3.1037880
H	-0.0015409	3.3765543	-1.3967785
H	0.0002967	3.3765774	1.3966449
H	-2.1485635	0.0294170	-4.9875662
H	-0.0029155	-0.3313543	-6.1618770
H	2.1436073	0.0358587	-4.9911263
H	-2.3950645	1.1304572	-1.3877327
H	-4.3645931	-0.2894642	-1.8472978
H	-2.8819851	-1.2747701	-1.8756167
H	-3.6755079	-0.8128806	-3.3950849
H	-4.3098554	2.1582746	-2.5589686
H	-3.6278258	1.7252548	-4.1384959
H	-2.7943912	2.9087420	-3.1121017
H	2.3931677	1.1292958	-1.3893149
H	2.8982658	-1.2687873	-1.8989056
H	4.3717973	-0.2704627	-1.8637020
H	3.6858944	-0.7865947	-3.4149848
H	4.2961696	2.1806897	-2.5610580
H	2.7723384	2.9240771	-3.1008613
H	3.6095372	1.7552821	-4.1406939
H	-2.1433197	0.0372271	4.9921368
H	0.0034863	-0.3299635	6.1621213
H	2.1488497	0.0314558	4.9878140
H	-2.3937178	1.1332446	1.3909357
H	-4.3682910	-0.2749942	1.8598061
H	-3.6801721	-0.7948296	3.4090261
H	-2.8909303	-1.2681042	1.8907659
H	-2.7802898	2.9203269	3.1088672
H	-3.6156101	1.7451214	4.1430068
H	-4.3010038	2.1743049	2.5640058
H	2.3948079	1.1378652	1.3892696
H	2.8741547	-1.2714229	1.8626247
H	3.6686131	-0.8214042	3.3852140
H	4.3604623	-0.2914196	1.8406731
H	4.3138156	2.1531908	2.5625235
H	3.6346909	1.7134437	4.1411053
H	2.8019512	2.9049551	3.1237055
Au	0.0002814	-1.5263122	0.0001920

Au(NHC) (**9**)
71
Energy = -1336.734702165

N	-0.0461473	1.1744443	1.3076889
C	-0.0323385	0.0000212	0.6711985
N	-0.0472269	-1.1741930	1.3081735
C	-0.0938378	-1.2469220	2.7910896
C	-0.7452652	0.0009380	3.3673341
C	-0.0923979	1.2477756	2.7902807
C	0.0110137	-2.4428282	0.5947934
C	-1.2025230	-3.0909665	0.2706257
C	-1.1158593	-4.3313177	-0.3750539
C	0.1166445	-4.9089931	-0.6700672
C	1.2953898	-4.2558559	-0.3204857
C	1.2759331	-3.0116058	0.3251474
C	-2.5730626	-2.5051532	0.5861251
C	-3.3798030	-3.4223641	1.5251228
C	2.5930428	-2.3496321	0.7096179
C	3.3465307	-3.1783106	1.7684581
C	0.0125373	2.4429811	0.5941724
C	-1.2010322	3.0918514	0.2718285
C	-1.1142768	4.3324850	-0.3733032
C	0.1184261	4.9093506	-0.6692256
C	1.2972342	4.2552625	-0.3216308
C	1.2776043	3.0107352	0.3234761
C	-2.5717215	2.5070143	0.5886253
C	-3.3749228	3.4220079	1.5328997
C	2.5946800	2.3475842	0.7060856
C	3.3534461	3.1788250	1.7590390
C	-3.3643652	-2.2050602	-0.7001240
C	3.4819135	-2.0959276	-0.5211031
C	-3.3668550	2.2132518	-0.6967529
C	3.4786424	2.0879150	-0.5269289
H	-0.6581631	-2.1518029	3.0476657
H	0.9334456	-1.3778768	3.1672105
H	-1.8216435	0.0013001	3.1415871
H	-0.6405319	0.0010731	4.4603754
H	-2.0326049	-4.8556909	-0.6477778
H	0.1583788	-5.8775141	-1.1695928
H	2.2543547	-4.7227624	-0.5484258
H	-2.4239963	-1.5466851	1.1071041
H	-4.3332902	-1.7462495	-0.4582093
H	-2.8132119	-1.5166024	-1.3578299
H	-3.5631105	-3.1236798	-1.2698472
H	-4.3368677	-2.9512676	1.7899725
H	-3.6063489	-4.3852068	1.0460965
H	-2.8354559	-3.6364122	2.4557830
H	2.3673903	-1.3680041	1.1548828
H	4.4040317	-1.5760303	-0.2262250
H	3.7750310	-3.0374352	-1.0061954
H	2.9647505	-1.4792103	-1.2705698
H	4.2645514	-2.6598982	2.0793978
H	2.7322405	-3.3546905	2.6627153
H	3.6379918	-4.1602426	1.3697831
H	-0.6555986	2.1533088	3.0470224
H	0.9350590	1.3773133	3.1665625
H	-2.0308937	4.8577765	-0.6446427
H	0.1602329	5.8780994	-1.1682961
H	2.2562310	4.7216944	-0.5503953

H	-2.4229423	1.5463093	1.1055222
H	-4.3354978	1.7542968	-0.4539317
H	-2.8184364	1.5271666	-1.3591545
H	-3.5664698	3.1344161	-1.2620241
H	-4.3324700	2.9517925	1.7974950
H	-3.6001035	4.3873160	1.0582735
H	-2.8284031	3.6312372	2.4634315
H	2.3687471	1.3680633	1.1558370
H	4.4017747	1.5685734	-0.2341758
H	3.7689663	3.0269794	-1.0183883
H	2.9575476	1.4683060	-1.2712596
H	4.2711050	2.6593370	2.0692684
H	2.7423803	3.3602068	2.6544972
H	3.6461083	4.1583732	1.3554244
Au	0.0084846	-0.0002337	-1.3226506

CyclododecyneAuCl (**6**)
34
Energy = -1065.679530633

Au	2.1458592	-2.9161983	2.6250636
Cl	3.0890264	-4.4633329	3.9804068
C	0.7908282	-1.4442423	1.8189912
C	1.7337920	-1.5645951	0.9987755
C	2.5787967	-1.4113903	-0.2035802
H	3.0907169	-2.3628770	-0.4080796
H	3.3735448	-0.6774437	0.0142118
C	1.1444688	0.4205976	-1.3141418
H	0.8015340	0.5602755	-0.2777116
H	1.9179472	1.1899217	-1.4792088
C	-0.0339219	0.6459709	-2.2677680
H	-0.7359217	-0.1993780	-2.1687168
H	0.3232743	0.6091403	-3.3108080
C	-0.7920779	1.9661774	-2.0543054
H	-0.1260915	2.8073153	-2.3123415
H	-1.6222493	2.0071820	-2.7797124
C	-1.3608237	2.2290755	-0.6458994
H	-1.8505910	3.2154834	-0.6795185
H	-0.5355272	2.3480057	0.0749407
C	-2.3849962	1.2067854	-0.1088582
H	-3.0412504	1.7195549	0.6149830
H	-3.0452902	0.8944536	-0.9354414
C	-1.8218092	-0.0517754	0.5814856
H	-2.6580938	-0.7414225	0.7860406
H	-1.1479404	-0.5950822	-0.0972404
C	-1.0981291	0.2359800	1.9014533
H	-1.8201067	0.6312169	2.6346510
H	-0.3375487	1.0208141	1.7677847
C	-0.4205741	-0.9992762	2.5350943
H	-0.1408566	-0.7721983	3.5753901
H	-1.1327315	-1.8395079	2.5907331
C	1.7608334	-0.9780404	-1.4393400
H	0.9625707	-1.7206802	-1.5991405
H	2.4164478	-1.0328578	-2.3226073

[CyclododecyneAuNHC(**7**)]$^{+}$ (**8**)
98
Energy = -1765.713859464

C	0.0927743	2.6970577	0.4253903
C	-0.2754250	2.6204581	-0.7625077
C	-0.6938235	2.8456358	-2.1564214
H	-1.2637045	3.7916347	-2.1718127
H	-1.4095140	2.0589242	-2.4368366
C	0.4443503	2.8989911	-3.2114377
H	1.1956391	2.1304931	-2.9762484
H	-0.0043189	2.6008624	-4.1705037
C	1.0995199	4.2767495	-3.4002240
H	1.7347529	4.2268250	-4.3001935
H	0.3058977	5.0057613	-3.6359187
C	1.9384265	4.8078716	-2.2279777
H	1.3236327	4.8158998	-1.3130260
H	2.1835613	5.8643386	-2.4257091
C	3.2422444	4.0353247	-1.9873219
H	3.0272903	2.9582265	-1.8895193
H	3.8763940	4.1270918	-2.8845217
C	4.0489646	4.5118303	-0.7661198
H	5.0066610	3.9661825	-0.7372738
H	4.3092892	5.5741587	-0.9025643
C	3.3339904	4.3483961	0.5862712
H	2.3881962	4.9132956	0.5570625
H	3.9370062	4.8275033	1.3741752
C	3.0662203	2.8865371	0.9748461
H	2.7353765	2.3200384	0.0889411
H	4.0106406	2.4173105	1.2929984
C	2.0241036	2.6911344	2.0820231
H	2.3258958	3.2247338	2.9970370
H	1.9643705	1.6242924	2.3472491
C	0.6041374	3.1865696	1.7175691
H	-0.0982282	2.9147525	2.5193210
H	0.5862612	4.2871257	1.6518452
C	-0.8124237	-1.4101450	0.3449407
C	-1.5263152	-3.5174878	-0.0493323
H	-1.9618707	-4.3257938	-0.6231047
C	-1.0286561	-3.4822901	1.2182776
H	-0.9442665	-4.2533384	1.9736622
C	-1.7894214	-1.8476628	-1.9096711
C	-0.8559366	-1.9886060	-2.9584016
C	-1.2732977	-1.6020980	-4.2395637
H	-0.5808188	-1.6970135	-5.0769387
C	-2.5567581	-1.1088648	-4.4635621
H	-2.8601425	-0.8199646	-5.4707295
C	-3.4585413	-0.9963773	-3.4075711
H	-4.4649771	-0.6218438	-3.5989363
C	-3.1014543	-1.3661505	-2.1032558
C	0.5456958	-2.5506428	-2.7578548
H	0.6756023	-2.7762432	-1.6890076
C	1.6290266	-1.5270743	-3.1420247
H	2.6295545	-1.9431315	-2.9575907
H	1.5299273	-0.6027520	-2.5553375
H	1.5718351	-1.2607100	-4.2070158
C	0.7324239	-3.8699528	-3.5313128
H	1.7266257	-4.2927655	-3.3290956
H	0.6513721	-3.7127988	-4.6162759
H	-0.0207911	-4.6173917	-3.2456770
C	-4.1255387	-1.2609053	-0.9803656
H	-3.6376632	-1.5621019	-0.0413239
C	-4.6213832	0.1841481	-0.7935883

H	-3.7886058	0.8688948	-0.5781762
H	-5.3318494	0.2378705	0.0432725
H	-5.1396638	0.5516667	-1.6907822
C	-5.3055054	-2.2237280	-1.2150540
H	-6.0087240	-2.1778380	-0.3715702
H	-4.9658969	-3.2635106	-1.3204010
H	-5.8602004	-1.9602470	-2.1268067
C	0.0148393	-1.7283034	2.6814121
C	1.4089709	-1.8813334	2.8371094
C	1.9677849	-1.4384770	4.0440030
H	3.0420173	-1.5402483	4.2032995
C	1.1765119	-0.8794108	5.0450180
H	1.6343519	-0.5457835	5.9771311
C	-0.1992872	-0.7577960	4.8645414
H	-0.8095681	-0.3321974	5.6621970
C	-0.8183867	-1.1831774	3.6808713
C	2.3017217	-2.5194098	1.7803702
H	1.6835282	-2.7452804	0.8987241
C	3.4178933	-1.5646415	1.3213280
H	4.0204720	-2.0351396	0.5316241
H	4.0972750	-1.3118076	2.1477207
H	3.0052609	-0.6270515	0.9232879
C	2.8891450	-3.8516977	2.2851772
H	2.1008277	-4.5558218	2.5860577
H	3.5436616	-3.6940112	3.1542170
H	3.4891583	-4.3279833	1.4968931
C	-2.3304072	-1.0679045	3.5356227
H	-2.6088418	-1.4401175	2.5384725
C	-2.8012737	0.3946730	3.6245604
H	-2.3282890	1.0141948	2.8488543
H	-2.5640717	0.8351614	4.6035311
H	-3.8904454	0.4539746	3.4899027
C	-3.0566943	-1.9454306	4.5730956
H	-4.1439309	-1.8962213	4.4195692
H	-2.8492865	-1.6072076	5.5982943
H	-2.7489811	-2.9978416	4.5005968
Au	-0.4249355	0.5616934	0.1117665
N	-1.3870850	-2.2392367	-0.5719972
N	-0.5937192	-2.1835857	1.4455047

[CyclododecyneAuNHC(**9**)]$^{+}$ (**10**)
103
Energy = -1806.234910835

C	0.8979335	0.5610857	-1.9858749
C	0.9692084	1.9775766	-2.3938997
H	-0.0480149	2.3370888	-2.6130558
H	1.3284510	2.5752891	-1.5406650
C	1.8903260	2.1967485	-3.6199428
H	1.4778282	1.6380552	-4.4721421
H	1.8306682	3.2631415	-3.8883901
C	3.3379407	1.7815840	-3.3398371
H	3.3165112	0.8092260	-2.8275381
H	3.7765342	2.4832506	-2.6107049
C	4.2853830	1.6775835	-4.5484367
H	4.5701319	2.6895014	-4.8799393
H	5.2196214	1.2164717	-4.1889617
C	3.7777045	0.9167022	-5.7898474
H	4.6322563	0.8000021	-6.4763759

H	3.0603227	1.5562897	-6.3308624
C	-1.1822927	0.0055081	1.6654958
C	-2.2759778	-1.2372200	3.5187287
H	-2.8921450	-2.1444455	3.4770072
H	-1.5659861	-1.3614842	4.3532424
C	-3.1323558	0.0059886	3.7070789
H	-3.9608293	0.0034715	2.9833207
H	-3.5745689	0.0071931	4.7119457
C	-1.1369333	-2.4262056	1.6527878
C	-2.0408445	-3.0639365	0.7717238
C	-1.6649639	-4.3067647	0.2439431
H	-2.3401075	-4.8222311	-0.4407106
C	-0.4531182	-4.9018565	0.5877814
H	-0.1866527	-5.8748811	0.1729474
C	0.4102626	-4.2625986	1.4740404
H	1.3496065	-4.7449938	1.7484378
C	0.0900896	-3.0166353	2.0319642
C	-3.3923347	-2.4698298	0.3951211
H	-3.4833106	-1.4928922	0.8930353
C	-3.5025970	-2.2186083	-1.1195042
H	-4.4678517	-1.7510821	-1.3604268
H	-2.7020061	-1.5534390	-1.4735472
H	-3.4393908	-3.1577431	-1.6877090
C	-4.5524551	-3.3555636	0.8894648
H	-5.5185841	-2.8795706	0.6690426
H	-4.5444515	-4.3369365	0.3942894
H	-4.4993438	-3.5326443	1.9730674
C	1.0494134	-2.3749850	3.0267032
H	0.6447604	-1.3890621	3.3009097
C	2.4403239	-2.1385504	2.4119553
H	3.0990259	-1.6401410	3.1369959
H	2.9211308	-3.0854441	2.1273017
H	2.3782740	-1.5051226	1.5154767
C	1.1562445	-3.2134036	4.3155743
H	1.8018544	-2.7096342	5.0490037
H	0.1730910	-3.3763206	4.7792274
H	1.5924412	-4.2016635	4.1112246
Au	-0.1443771	-0.0066904	-0.0982211
N	-1.5202132	-1.1585310	2.2494750
C	1.0066894	-0.6769674	-1.8807638
C	1.2938307	-2.1140214	-2.0507288
H	0.3476682	-2.6731946	-1.9865655
H	1.9088697	-2.4591519	-1.2039939
C	2.0021607	-2.4226013	-3.3914134
H	1.3925345	-2.0012619	-4.2040865
H	1.9821498	-3.5145099	-3.5288679
C	3.4496553	-1.9053352	-3.4717540
H	3.5490557	-1.0071576	-2.8436309
H	4.1272933	-2.6517391	-3.0276497
C	3.9161379	-1.5738916	-4.9018627
H	3.8631544	-2.4937908	-5.5055521
H	4.9833433	-1.3031424	-4.8728959
C	3.1028782	-0.4557097	-5.6000744
H	2.8075461	-0.7989104	-6.6032411
H	2.1510854	-0.3130783	-5.0626218
C	-2.2793022	1.2508884	3.5143098
H	-2.8978647	2.1562380	3.4697774
H	-1.5693179	1.3798333	4.3481236
C	-1.1415025	2.4371488	1.6465140

C	-2.0491242	3.0745687	0.7693470
C	-1.6758430	4.3170629	0.2397169
H	-2.3538653	4.8325833	-0.4422041
C	-0.4617743	4.9110600	0.5765688
H	-0.1957941	5.8829485	0.1586616
C	0.4056451	4.2719687	1.4590687
H	1.3470718	4.7535632	1.7276037
C	0.0870951	3.0271964	2.0203616
C	-3.4014907	2.4789120	0.3987326
H	-3.4911352	1.5041727	0.9012436
C	-3.5152166	2.2201631	-1.1143047
H	-4.4821587	1.7544898	-1.3518360
H	-2.7176483	1.5497419	-1.4654449
H	-3.4493942	3.1563458	-1.6870854
C	-4.5610205	3.3666282	0.8905790
H	-5.5274127	2.8902036	0.6722812
H	-4.5531153	4.3461824	0.3919391
H	-4.5071047	3.5475672	1.9734266
C	1.0493895	2.3864626	3.0124637
H	0.6494602	1.3975851	3.2831649
C	2.4412484	2.1594913	2.3964030
H	3.1000234	1.6540594	3.1164879
H	2.9207241	3.1104021	2.1234018
H	2.3811497	1.5384226	1.4913542
C	1.1516809	3.2205882	4.3045982
H	1.7995314	2.7174352	5.0364986
H	0.1677416	3.3773981	4.7688132
H	1.5830646	4.2116033	4.1035758
N	-1.5229720	1.1701877	2.2454257