Electronic Supplementary Material (ESI) for Chemical Communications


# Electrochemistry of $Au^{II,III}$ Pincer Complexes: Determination of the $Au^{II}$–$Au^{II}$ Bond Energy

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**SUPPORTING INFORMATION**

## Experimental Section

### Synthesis

All manipulations were performed using standard Schlenk techniques under dry nitrogen or a Saffron Scientific glove box. Nitrogen was purified by passing through columns of supported $P_2O_5$, with moisture indicator, and activated 4 Å molecular sieves. Anhydrous solvents were freshly distilled from appropriate drying agents. LAuCl,[S1] LAuOH[S2], LAuH[S3] and LAuAuL[S3]([L = 2,6-$(C_6H_3Bu^t)_2$-pyridine) were prepared using literature methods.

### Electrochemistry

All electrochemical measurements were performed under an inert atmosphere using an Autolab PGSTAT 302N computer-controlled potentiostat. Cyclic voltammetry (CV) was performed using a three-electrode configuration comprising of a Pt wire counter electrode (GoodFellow, Cambridge, UK; 99.99%), a Ag wire pseudoreference electrode (GoodFellow, Cambridge, UK; 99.99%) and either a glassy carbon (GC) macrodisk working electrode (Bioanalytical Systems, Indiana, USA; 3mm diameter) or a Pt microdisk working electrode (GoodFellow, Cambridge, UK; 99.99%; radius 19.0 ± 0.5 µm. The GC working electrode was polished between experiments using successively fine grades of diamond slurry (3-0.25 µm), rinsed in ethanol and subjected to brief ultrasonication to remove any adhered diamond particles. The Pt working electrode was polished between experiments using alumina slurry (0.3 µm), rinsed in distilled water and subjected to brief ultrasonication to remove any adhered alumina microparticles. The electrodes were then dried in an oven at 120 °C to remove any residual traces of water. The working electrode area was calibrated before each experiment using a 5.0 mM solution of ferrocene in $CH_3CN$ solvent containing 0.1 M $[nBu_4N][PF_6]$ as the supporting electrolyte. The GC macrodisk working electrode area was accurately determined by construction of a Randles–Sevcik plot of peak current vs. the square root of the voltage scan rate obtained from cyclic voltammograms recorded at varying scan rates from 50 to 750 mV $s^{-1}$. The Pt microdisk working electrode area was accurately determined using the steady–state

current measured using linear sweep voltammetry (scan rate = 10 mV $s^{-1}$).[S4] The Ag wire pseudo–reference electrode was calibrated to the ferrocene/ferrocenium couple in $CH_2Cl_2$ at the end of each run to allow for any gradual drift in potential, following IUPAC recommendations.[S5] All electrochemical measurements were performed at ambient temperatures under an inert $N_2$ atmosphere in $CH_2Cl_2$ containing 0.05 M [$^n$Bu$_4$N][B(C$_6$F$_5$)$_4$] as the supporting electrolyte, and iR-compensated using positive-feedback to within 85 ± 5% of the uncompensated solution resistance. The weakly coordinating electrolyte [$^n$Bu$_4$N][B(C$_6$F$_5$)$_4$] was prepared by literature methods.[S6] Data were recorded with Autolab NOVA software. CV simulations were performed using DigiElch – Professional (v 7.030) software.

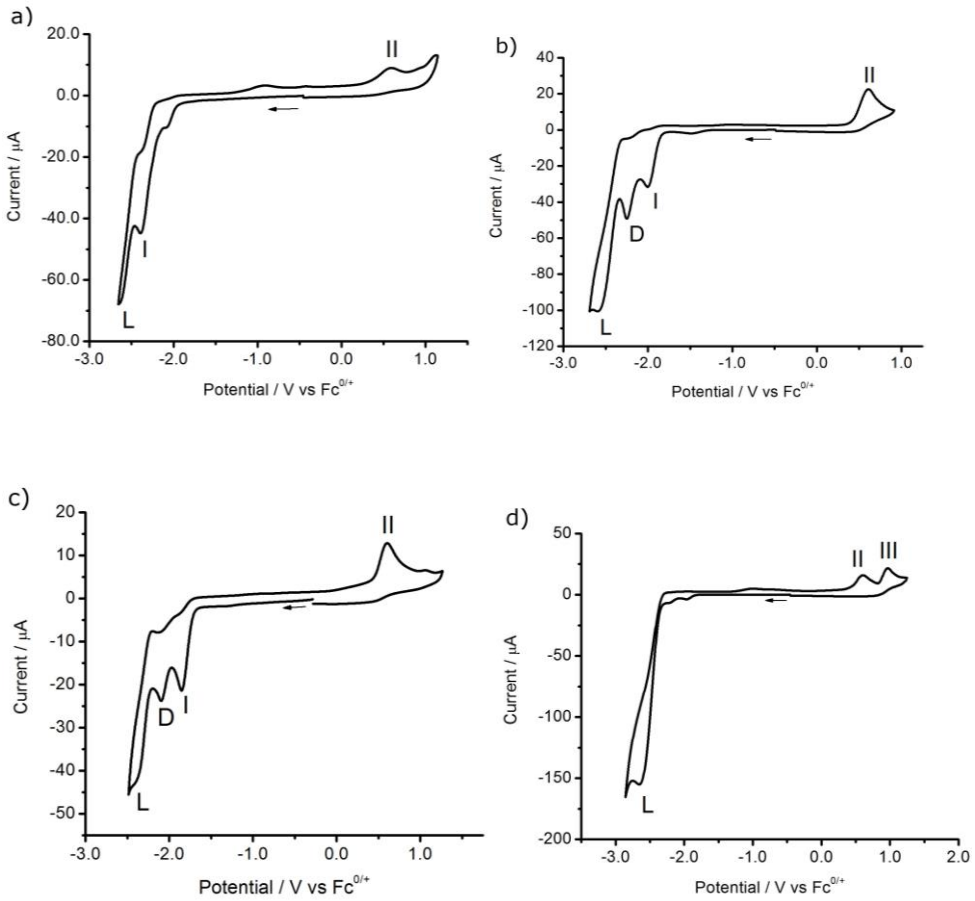


**Figure S1.** Full range cyclic voltammograms of **1** (a), **2** (b), **3** (c) and **4** (d) in $CH_2Cl_2$ (1.5 mM, 0.05 M [*n*Bu$_4$N][B(C$_6$F$_5$)$_4$]) at a scan rate of 100 $mVs^{-1}$.

**Digital simulation of cyclic voltammetry**

In order to obtain kinetic and thermodynamic parameters for the electrochemical processes observed, and to support the proposed mechanisms postulated above, digital simulations were performed for the metal centered reductions of **1** and **2** and the oxidation of **4**.

Diffusion coefficients, *D*, were first estimated by application of the Randles-Sevcik method for **1** and **2**, in which the peak current for the reduction is plotted vs. the square root of scan rate. This assumes a single electron transfer (n = 1). These values gave a starting point for the simulations and produce values for the diffusion coefficients of **1**, **2** and **4** that are in good agreement with those obtained from DOSY experiments. The diffusion coefficient for **4** was determined by performing potential-step chronoamperometry at a microdisk electrode. The current transients (*i*) were then fitted using the empirical procedure of Shoup and Szabo,[S7] which describes the current transient at a microelectrode on both short ($\tau < 1$) and long ($\tau > 1$) timescales according to equation 1:

$$i = 4nFC^*Drf(\tau) \qquad (1)$$

in which *n* is the number of electrons transferred, *F* is the Faraday constant (96 485 C $mol^{-1}$), *C** is the bulk concentration (mM), D is the diffusion coefficient ($m^2s^{-1}$), *r* is the radius of the electrode (m), and f(τ) is given by:

$$f(\tau) = 0.7854 + 0.8863\tau^{-1/2} + 0.2146\exp(-0.7823\tau^{-1/2}) \qquad (2)$$

where $\tau \equiv 4Dt/r^2$ is the dimensionless time. The Shoup-Szabo best fit simultaneously gives optimized parameters for D and nC* (Figure S2). As C* is known, the other parameters can then be deduced. The Shoup-Szabo best fit for **3** yielded a value for the diffusion coefficent of 7 ± 1 x $10^{-6}$ $cm^2s^{-1}$ and gave the number of electrons transferred during the oxidation of the dimer, *n*, as being equal to 1.

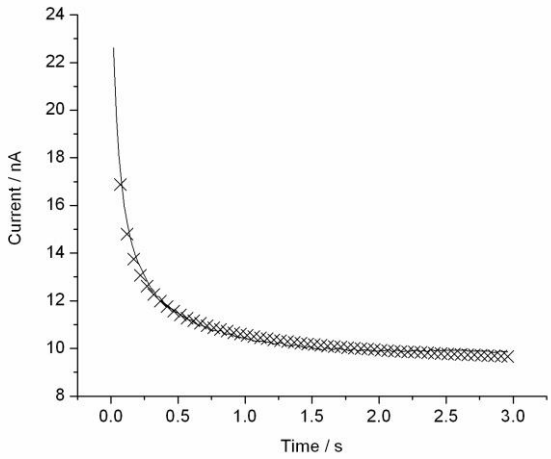


**Figure S2**: Experimental chronoamperogram (solid line) and Shoup–Szabo best fit (crosses) for the reduction of 1 in $CH_2Cl_2$ (1.5 mM, 0.05 M [$n$Bu$_4$N][B($C_6F_5$)$_4$]) at a 19 µm radius Pt microdisk.

**Cyclic voltammograms at varying weep rates:**

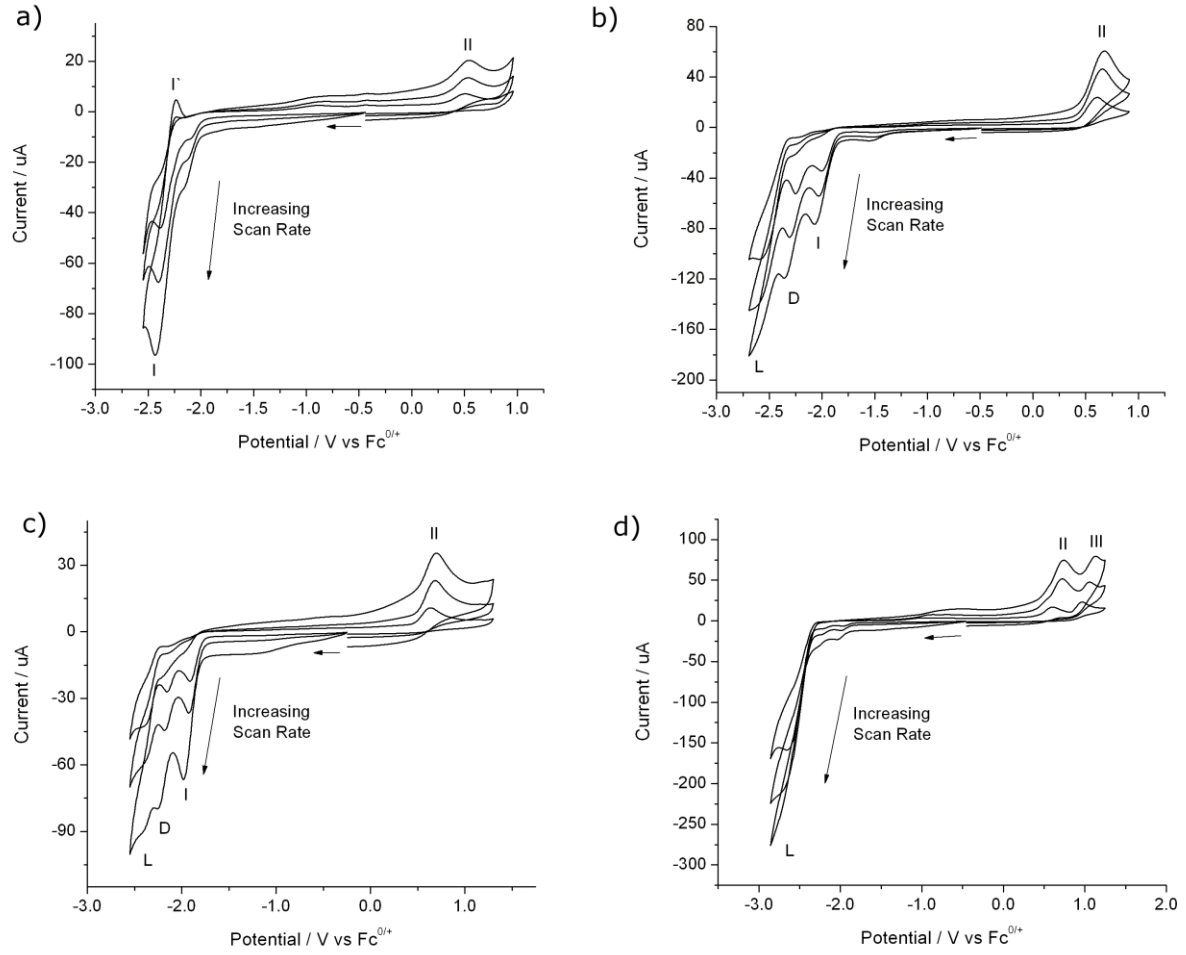


**Figure S3:** Overlaid reductive cyclic voltammograms of **1** (a), **2** (b) 3 (c) and 4 (d) in $CH_2Cl_2$ (1.5 mM 0.05 m [$n$Bu$_4$N][B(C$_6$F$_5$)$_4$]) at scan rates of 50-1000 $mVs^{-1}$. Note that a small reduction wave observed before the main wave (I) in figure a) is due to the presence of trace **2** impurity arising from the synthesis of **1** (see reference S3).

**DFT calculations**

To reduce computational complexity, simulations were performed using modified ligand structures in which the t-Bu group were replaced by a hydrogen atom. Initial geometries were derived from X-ray data, where available, with appropriate manual modification. All calculations were performed using the Gaussian 09 software package.[S14] Geometry optimisation and frequency calculations were carried out using the pure functional of Perdew, Burke and Ernzerhof[S15,16] made into a hybrid by Adamo,[S17] using 25% exchange and 75% correlation weighting ('PBE0'). Gold atoms were described using the def-TZVP basis set;[S18,19] all other atoms were described using the TZVP basis set.[S20,21] Structures were geometry optimised in the gas phase with the default convergence criteria and confirmed as minima

through frequency calculations. Zero-point energies and theromodynamic properties were calculated at 298.15 K and 1 atm. Bond enthalpies were calculated from the difference in energy of complete molecules and the sum of the energy of the appropriate optimised fragments obtained by homolytic bond cleavage. Final atomic coordinates for the optimised structures are given in the appendix.

The electrochemical process was modelled for the following steps, using $NMe_4^+$ ions to take account of the presence of supporting electrolyte and counterbalance the charges (Table S3).

a) $2(C\text{^}N\text{^}C)Au^{III}\text{-}X + 2\ NMe_4^+$
b) $\{NMe_4^+[(C\text{^}N\text{^}C)Au^{II}\text{-}X^-]\} + (C\text{^}N\text{^}C)Au^{III}\text{-}X + NMe_4^+$
c) $(C\text{^}N\text{^}C)Au^{II\bullet} + NMe_4^+\ X^- + (C\text{^}N\text{^}C)Au^{III}\text{-}X + NMe_4^+$
d) $(C\text{^}N\text{^}C)Au^{II}\text{-}X\text{-}Au^{III}(C\text{^}N\text{^}C) + \{NMe_4^+\ X^-\} + NMe_4^+$
e) $\{\ NMe_4^+\ [(C\text{^}N\text{^}C)Au^{II}\text{-}X\text{-}Au^{II}(C\text{^}N\text{^}C)]\} + \{NMe_4^+\ X^-\}$
f) $(C\text{^}N\text{^}C)Au^{II}\text{-}Au^{II}(C\text{^}N\text{^}C) + 2\{NMe_4^+\ X^-\}$

**Table S3**. Calculated relative energies (kJ $mol^{-1}$) of processes (a) to (f).

| | X = H | X = OH |
|---|---|---|
| (a) | 0 | 0 |
| (b) | -410 | -444 |
| (c) | -169 | -475 |
| (d) | -217 | -495 |
| (e) | -740 | -1054 |
| (f) | -563 | -1174 |

For X = OH the optimized geometry of $(C\text{^}N\text{^}C)Au^{II}\text{-}X\text{-}Au^{III}(C\text{^}N\text{^}C)$ is highly asymmetric, and a reduced hydroxide-bridged dimer $[(C\text{^}N\text{^}C)Au^{II}\text{-}OH\text{-}Au^{II}(C\text{^}N\text{^}C)]^-$ could not be modelled: the energy given for this case is that of the $\{(C\text{^}N\text{^}C)Au^{II}\text{-}OH\cdots\ Au^{II}(C\text{^}N\text{^}C)\}^-$ assembly.
The relative energy profile for the reduction processes for $(C\text{^}N\text{^}C)Au^{III}\text{-}H$ and $(C\text{^}N\text{^}C)Au^{III}\text{-}OH$ are shown in Figure S5.

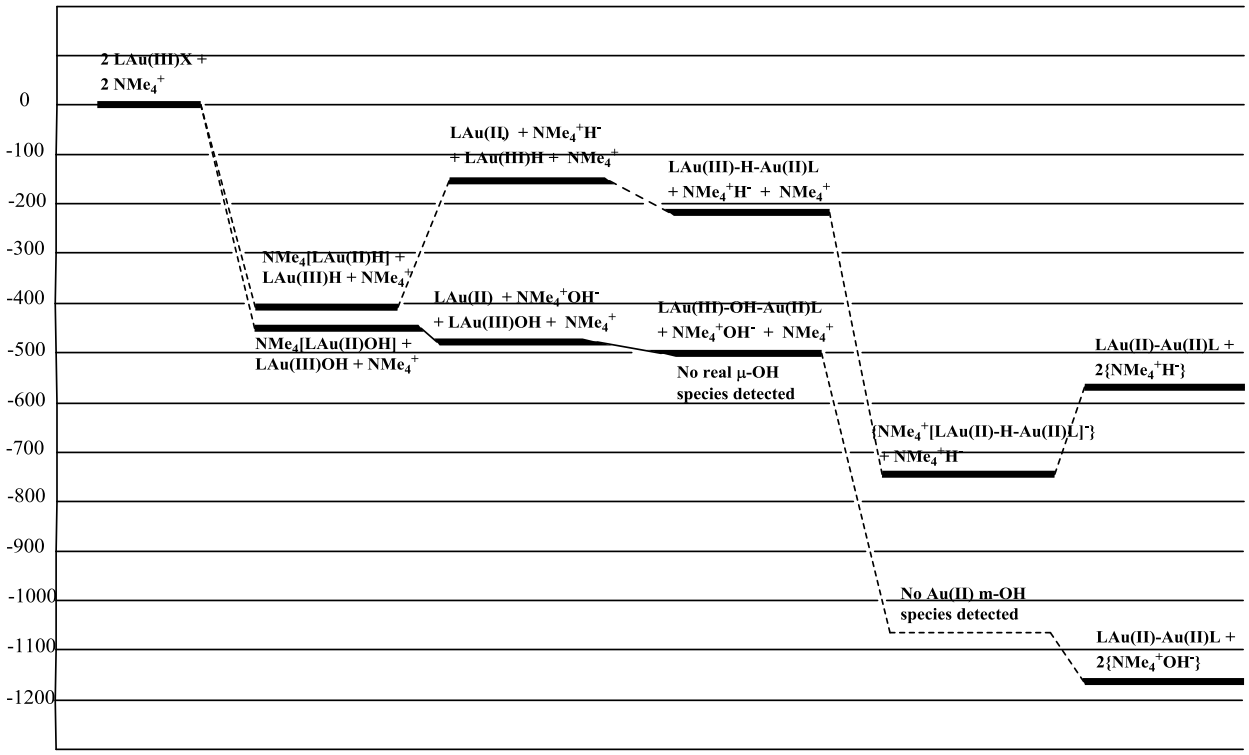


**Figure S5**. Calculated energy profile for the electrochemical reduction of (C^N^C)$Au^{III}$-H and (C^N^C)$Au^{III}$-OH. $NMe_4^+$ cations are included to take account of the presence of supporting electrolyte.

Note that these calculated values are strictly the internal energy of the system, which in a closed system at constant pressure and volume we can approximate to the bond enthalpy if entropic contributions are neglected.

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**Appendix: DFT Coordinates**

**(C^N^C)Au-H**

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**(C^N^C)Au-OH**

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**{(C^N^C)Au-H···NMe4}**

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**{(C^N^C)Au-OH···NMe4}**

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H -4.464867466845 -1.038188637579 -1.397642725230
H -4.481607599218 1.209469316444 -1.315043562694
H -4.561302174442 3.544086353767 -0.559777097664
N -1.229290524434 -1.154212515042 -0.522019552828
Au 0.015301248856 -0.090077273822 0.622620312658
H -2.710323451711 4.484295254305 0.795664390034
H 3.858933883758 -3.719967707758 1.280343252966
N 3.089980343389 2.272510704131 -1.063753414295
C 3.175896507746 0.780321675400 -1.027356880110

H 2.668990461494 0.376679330836 -1.902385731301
H 4.228033205958 0.496740121121 -1.037519713857
H 2.690202050772 0.437986817736 -0.112704229631
C 3.685550988909 2.811380614105 0.192697866888
H 4.728903852984 2.501095514161 0.244856883368
H 3.618576868528 3.898882040318 0.171722465427
H 3.101847990898 2.390974998872 1.017952363770
C 1.656396835370 2.692362019682 -1.127641187513
H 1.620241813150 3.778433054936 -1.209200086319
H 1.193677161816 2.233955649897 -2.000162159304
H 1.166545661719 2.354679742521 -0.213367814839
C 3.818310865724 2.789242994263 -2.245866279979
H 3.363617401266 2.381517068760 -3.147790872733
H 3.753533379953 3.876585913538 -2.259095821778
H 4.861437488593 2.480912037669 -2.186604109274
O 1.477450037339 1.132073821493 1.504035138064
H 1.326882362745 1.067929030051 2.449978683006

**(C^N^C)Au**

C 2.456508792952 6.784695322590 -1.976338919891
C 3.492337365285 5.884030107350 -1.769612988991
C 1.146943595677 6.432157940237 -1.663922692365
C 3.214852267301 4.630536249487 -1.249908332005
C 0.831346951294 5.183653491121 -1.140988759859
C 1.903466561955 4.274238925776 -0.935876566063
C 1.587251533301 2.943947739477 -0.381401303093
C 2.456429031127 1.891898338399 -0.094313548722
C -2.382098049271 2.943552044380 0.155280458674
C -3.761045863626 3.010668918508 0.315849191880
C -0.277392093179 1.644096216469 0.370723356152
C 1.927398136353 0.719528109135 0.428238930774
C -1.741089795100 1.733518857091 0.534136158539
C 0.567559780072 0.575157015594 0.667684502534
C -4.491105500317 1.941216136205 0.825912499139
C -2.475517614259 0.663482034825 1.044926701781
C -3.849005434590 0.765989671035 1.191141499933
H 4.513105237445 6.157060467382 -2.012337985379
H 0.356596814243 7.155965075195 -1.835710127775

H 4.029734487386 3.931705618155 -1.090956264820
H 3.519180384253 1.984391521551 -0.273650227308
H -4.288830572943 3.917589689508 0.038333211300
H 2.594061040980 -0.105341000166 0.655364951893
H 0.175106087415 -0.346742270034 1.075402578875
H -1.980435741764 -0.258393139607 1.332500907846
H -4.416181791820 -0.068143589885 1.588578132429
N 0.293202630297 2.741596427162 -0.128565633895
Au -1.003920296589 4.346362760239 -0.570758045694
H -5.567275730993 2.025958956117 0.938830609435
H 2.669405427115 7.768061786703 -2.383454285325

**(C^N^C)Au-H-Au(C^N^C)**

C -4.290395900661 4.818236997035 -3.278179444251
C -1.899844485053 3.159421400215 -4.247840032128
C -5.407048051405 5.422276827500 -2.717204360778
C -0.835690353710 2.361783259601 -4.635960295952
C -3.891652422059 3.575113808837 -2.789782974362
C -2.750835525277 2.746165079826 -3.223010683826
C -6.122556201393 4.818249120273 -1.692679822022
C -0.619172499248 1.147827590767 -3.998405391495
C -2.541784211245 1.506419127520 -2.563646813387
C -5.695831193181 3.575624640656 -1.227187317150
C -1.465744370051 0.730961296126 -2.975352473881
C -6.728921516712 -4.947080194058 -0.682825366125
C -5.531576748968 -5.325843333145 -0.097850704032
C -6.912474806853 -3.629755479962 -1.080326836750
C -2.832288526398 -6.014908598555 1.184997320088
C -1.563709227576 -6.141209731947 1.733839433567
C -4.514438510002 -4.390328033775 0.090510183255
C -3.229490014080 -4.766019168391 0.710244494715
C -6.286715950737 2.747969047875 -0.158469826673
C -5.900377981211 -2.692575412670 -0.894706510381
C -4.688339820163 -3.040276359925 -0.312668344074
C -0.696826295497 -5.060447820698 1.817000809980
C -7.414413961923 3.167996589750 0.546600884462
C -1.126284761670 -3.825548884236 1.333791359533
C -5.670923256245 1.503006115118 0.135322266078

C -0.391942962249 -2.546220078967 1.314506723112
C -1.043543781406 -1.414143157100 0.758385336604
C 0.901880165530 -2.443082338600 1.825028528632
C -7.949587485132 2.371729416274 1.546015101099
C -6.232342986561 0.727997291541 1.141728933266
C -0.346716928031 -0.212955375860 0.742159374266
C 1.569597232982 -1.229602557770 1.794965971058
C 0.944432645300 -0.115159173300 1.252532066242
C -7.357991652720 1.151365712542 1.842287633495
H -3.744361180630 5.303706694957 -4.075895404098
H -2.061951057838 4.107070847045 -4.751359878090
H -5.728259115461 6.389553119792 -3.088391639060
H -0.177180959099 2.687247078516 -5.433497655934
H -6.990949612531 5.303304902939 -1.267466850659
H -7.516484097750 -5.678144241961 -0.827457435924
H -5.396324474286 -6.357667418350 0.210201326143
H -3.494991202576 -6.868028834620 1.128432528266
H -1.275241285417 -0.220071885727 -2.488161779608
H -1.242025755073 -7.107732108767 2.106576710657
H -7.883041268861 4.120593807672 0.321225955253
H -6.067203294608 -1.667303993774 -1.209492923022
H 0.288747978640 -5.177191101384 2.247356584744
H 1.397827359750 -3.309448206806 2.250814481488
H -8.826133471388 2.702855961726 2.091582122240
H -0.814662266284 0.670415410435 0.319326597224
H 2.575155261157 -1.154416131345 2.193489320452
H -5.788534719722 -0.231538665081 1.387550941280
Au -3.993270129106 1.164306826539 -1.083530216327
Au -2.979086053875 -1.887110366821 0.091457911406
N -4.615989784815 3.040225534777 -1.803070259820
N -2.355906351493 -3.761004925883 0.815898023907
H 1.464787866436 0.836989403454 1.225980347538
H 0.214260677078 0.520743095289 -4.298772879970
H -7.775124919942 0.524118203064 2.623710791966
H -7.849634130846 -3.328884203179 -1.537794867670
H -3.486442577853 -0.362366615001 -0.498364194566

**(C^N^C)Au-OH-Au(C^N^C)**

C -4.719409027519 3.992924852177 -3.962801964145
C -2.023857640034 2.551149592691 -4.059303387750
C -5.973849275306 4.550481546886 -3.754137527098
C -0.803288149743 1.896084442613 -4.044061879587
C -4.217898698176 3.111779995804 -3.003550208350
C -2.915436822219 2.409334363560 -2.995416335537
C -6.723279921967 4.256705862145 -2.622635644979
C -0.472528885950 1.094230548934 -2.960276063206
C -2.596542442591 1.591668373723 -1.877478952028
C -6.188368037150 3.371409012107 -1.686103782539
C -1.361507301991 0.950104400945 -1.899339563210
C -6.666382553875 -4.182984779121 -0.537729779826
C -5.420578660718 -4.781121387842 -0.445374894340
C -6.823403553587 -2.845334332215 -0.193114390287
C -2.559800449341 -5.891404724839 -0.146895797057
C -1.227228909841 -6.220739323545 0.043721037302
C -4.326948265358 -4.035067353739 -0.005181915483
C -2.978416960975 -4.591782007242 0.120704651139
C -6.781106462849 2.920736998353 -0.407627497418
C -5.736920465918 -2.095729132018 0.248800771568
C -4.485145255319 -2.676458720640 0.347477645314
C -0.313454439738 -5.280805713049 0.496142701579
C -8.050887379023 3.345201910003 -0.014971925799
C -0.751598463424 -3.986951150050 0.756332123858
C -6.018565514947 2.048616537274 0.413570847081
C 0.041079228108 -2.848179478908 1.235156407411
C -0.646788812966 -1.626912190623 1.430566638271
C 1.409981189338 -2.942413364022 1.484746313262
C -8.588869867477 2.923466930135 1.190290408637
C -6.588927220296 1.648143477306 1.617672081639
C 0.081322018636 -0.531227446393 1.866668350118
C 2.110813440433 -1.832452936353 1.926373841763
C 1.447323343970 -0.627256128381 2.115090731865
C -7.854944046123 2.074588604703 2.008300014385
H -4.148685252139 4.242115750334 -4.847513966504
H -2.276355876440 3.174147822081 -4.911631937895
H -6.375700334240 5.238346030435 -4.490591580346
H -0.114916041783 2.010284244188 -4.874277661655

H -7.695171997883 4.708808022551 -2.474637989354
H -7.517607717886 -4.759866092287 -0.881184849784
H -5.308607333540 -5.825397794597 -0.718502558823
H -3.268301860810 -6.629101460111 -0.498130980603
H -1.075388590872 0.314609160839 -1.066145795435
H -0.893368571497 -7.231564004075 -0.162769120876
H -8.631444679184 4.008623606046 -0.648456804796
H -5.868165959796 -1.050882351672 0.510770280582
H 0.724437667103 -5.545745050477 0.644385879266
H 1.937584436541 -3.878612737039 1.335106019104
H -9.576331381631 3.257048432829 1.489918146334
H -0.406604794257 0.427796911637 2.014590857510
H 3.174840006060 -1.905902339150 2.119934220657
H -6.028646008952 0.984768208486 2.270358111868
Au -4.152872635271 1.561915890206 -0.445583411141
Au -2.675502490812 -1.851322151322 0.951528126363
N -4.986740836203 2.862027832552 -1.946916116788
N -2.053961725081 -3.710887709061 0.553623010348
H 1.996865560904 0.244117074566 2.455563841241
H 0.482827130310 0.578434559022 -2.940832357745
H -8.270773819803 1.744633656688 2.955578097085
H -7.800488579535 -2.379863209034 -0.270302377587
O -3.398192349459 -0.019477345417 1.319735899193
H -2.718500999906 0.490555161405 1.771619043227

**{(C^N^C)Au-H-Au(C^N^C)···NMe4}**

C 5.998827941181 -1.188535784435 0.850601022478
C 3.975737152759 -3.328197284377 1.711651409139
C 6.761563531223 -0.143593642225 0.340377639358
C 3.022211256643 -4.253650665969 2.107825251027
C 4.638198145997 -1.214463095306 0.543452972226
C 3.610069376428 -2.192677209805 0.987951270823
C 6.197391915680 0.862579506986 -0.433212230609
C 1.691530388744 -4.049623072194 1.768936013551
C 2.246214415856 -1.952108292147 0.651224721395
C 4.830108963898 0.790928778236 -0.710922508754
C 1.320978180394 -2.914250355405 1.051849900503
C -3.422085312982 -4.041483459372 -2.156546298706

C -4.189033864662 -3.025727028344 -1.608237923553
C -2.042761263623 -3.897185258210 -2.215626306219
C -5.693711167381 -0.924628472733 0.050154847561
C -6.226272395116 0.164791948776 0.728914869439
C -3.588553809615 -1.864735303435 -1.118977447204
C -4.414682086485 -0.797597774364 -0.498030963726
C 3.991389109873 1.754094830096 -1.465246736007
C -1.439287468400 -2.741374918634 -1.729406377703
C -2.173428546114 -1.696942141871 -1.170428059938
C -5.489240168177 1.330226185555 0.915013070701
C 4.573227251227 2.835104994920 -2.128210236939
C -4.218930338360 1.397511596862 0.340634766448
C 2.580406911988 1.558701195388 -1.495648909447
C -3.197043997161 2.463639005089 0.530601995896
C -1.824303349542 2.153684048241 0.287973477291
C -3.576569434344 3.728791641306 0.982356190395
C 3.789284405276 3.738617384111 -2.827671087117
C 1.826387483536 2.485188960416 -2.208779557825
C -0.908318644822 3.184226035488 0.508702616401
C -2.630455478137 4.719308284391 1.199313386536
C -1.291026475792 4.445258678194 0.957823200611
C 2.413219926698 3.561720169505 -2.867223548424
H 6.457568671974 -1.948676493668 1.469982126053
H 5.017598331797 -3.507557570067 1.958659858881
H 7.822098128144 -0.104385294982 0.566438088764
H 3.320449715698 -5.138446270266 2.659787811691
H 6.807183256170 1.679315254200 -0.797655563814
H -3.899318595615 -4.934683489346 -2.545284538322
H -5.269765485372 -3.131525954390 -1.583550340676
H -6.247787557393 -1.852671483107 -0.018414373554
H 0.279032883655 -2.787517908258 0.768054507049
H -7.217296092572 0.087190848756 1.164234321704
H 5.649966513007 2.973180364626 -2.111460440999
H -0.358781058570 -2.649695229148 -1.793467597055
H -5.888570329845 2.142556367072 1.510242890251
H -4.626712214393 3.955208365279 1.142154846639
H 4.251626106222 4.572830909303 -3.344032134963
H 0.145740698490 3.001093449391 0.314396389037

H -2.940014987042 5.703114496254 1.535581325475
H 0.748497851616 2.364581716162 -2.255621628544
Au 1.982544657349 -0.173509334062 -0.467876745702
Au -1.521905181983 0.189322075697 -0.479979179876
N 4.157000608835 -0.247270229527 -0.227641104465
N -3.795166576195 0.372743061304 -0.388399089676
H -0.543105223164 5.218332001541 1.108089379250
H 0.942558888424 -4.785563890353 2.047550992530
H 1.792422026941 4.263901713741 -3.415190237173
H -1.433423063727 -4.686672067976 -2.645333068086
C -1.246827260179 -1.060139278894 2.966081081363
H -2.099105023404 -1.346689815796 3.581563253841
H -1.567073255426 -0.787984398542 1.955815060370
H -0.522961153843 -1.871344568799 2.904820307790
C 0.551783284489 0.559607143947 2.718592491962
H 1.045254860502 1.406087109499 3.194741165580
H 1.240895562960 -0.273685825202 2.588281276879
H 0.145498579727 0.845368421239 1.747392216518
C -1.564541760165 1.235423898575 3.710565234311
H -2.394459131158 0.905387892146 4.334454748941
H -1.068070377319 2.091719882408 4.165172427307
H -1.912631679842 1.502442831733 2.711664986159
C -0.066910591391 -0.249059334511 4.929204645213
H -0.896914797666 -0.579517831430 5.552881071788
H 0.657949464834 -1.054015609002 4.816503273272
H 0.411931332794 0.620397781314 5.377908279644
N -0.582522790538 0.121921927963 3.588910097911
H 0.299046094259 -0.037955729173 -0.526712876878

**{(C^N^C)Au···HO-Au(C^N^C)···NMe4}**
C 6.507230117705 -0.492789489115 2.155550295821
C 4.889894053305 1.085018439900 4.243196467646
C 7.066307363539 -1.351485432240 1.214705982867
C 4.140941596876 2.024714238329 4.934660551842
C 5.152013488331 -0.645142343121 2.459982200725
C 4.313603899861 0.310963472623 3.235154630412
C 6.274587468235 -2.266045021263 0.528328109520
C 2.803218603688 2.196980052630 4.608261374049

C 2.937866712483 0.467361266404 2.878637173755
C 4.926400345907 -2.364286002088 0.882596279720
C 2.225900936530 1.429467155738 3.600797313798
C -3.031449130439 -3.276444546945 2.468893469262
C -4.044883880404 -2.612079163792 1.798976028792
C -1.718075536491 -2.841765206768 2.341596354294
C -6.137072089020 -1.012861052612 0.220481273527
C -6.943579515923 -0.192869842255 -0.551149729637
C -3.742261699682 -1.510257982423 0.997917572659
C -4.766278651703 -0.770115465868 0.258835380808
C 3.869832208317 -3.086632502246 0.121756177730
C -1.410135457352 -1.741467497316 1.546642754037
C -2.405835051754 -1.061934462597 0.864656597211
C -6.407920986754 0.858502932535 -1.280898435343
C 4.198635204385 -4.222491700081 -0.618988112035
C -5.037405907022 1.083489000459 -1.227667378306
C 2.542098749406 -2.556158334996 0.110090140249
C -4.270426500123 2.129960037978 -1.914116026922
C -2.875931617756 2.140388140944 -1.688887983141
C -4.861579256136 3.079933360539 -2.747358499691
C 3.243984596164 -4.873736391654 -1.384792236871
C 1.616819945247 -3.243945007853 -0.679686830695
C -2.113366294381 3.116312476908 -2.307254266029
C -4.076781597049 4.044243889292 -3.358127457203
C -2.704423293771 4.063740472547 -3.137079907749
C 1.948426170835 -4.377999174608 -1.415548621247
H 7.099724789474 0.296357224342 2.603689712181
H 5.931847883095 0.932512141690 4.511041010656
H 8.117733498582 -1.257565450234 0.962097395482
H 4.595364910792 2.608430863923 5.728243503950
H 6.686845563609 -2.850808111791 -0.285694477263
H -3.265057874037 -4.133585075083 3.090332848517
H -5.068257056184 -2.957665662987 1.903536178546
H -6.560310839881 -1.831312223801 0.786491989015
H 1.175922513390 1.587113421989 3.371144489098
H -8.011860370497 -0.376141892397 -0.586030947842
H 5.208720543021 -4.620528721914 -0.575904574787
H -0.369221527818 -1.426608500338 1.469397766089

H -7.042743807459 1.494904060587 -1.882195431635
H -5.932257151361 3.075545364983 -2.924183060152
H 3.507645530945 -5.765799423835 -1.943137801755
H -1.042107724228 3.136003387716 -2.131826905142
H -4.535230789011 4.783328828577 -4.005394673483
H 0.592234144666 -2.885577414810 -0.722626132838
Au 2.280522099614 -0.908817093872 1.410741817979
Au -2.314569852187 0.593507613638 -0.402927765946
N 4.470220617613 -1.641201301911 1.901403828577
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H 2.204437378178 2.928156794056 5.143864532991
H 1.190226314568 -4.878651667254 -2.010880891384
H -0.920388450980 -3.360830620263 2.862471552732
O -0.370537813794 0.996947649521 -0.426837661191
H 0.092073419809 0.390945068192 0.174626295510
C 2.380983621477 2.373194048888 -0.207127806880
H 1.383804817806 2.635554388213 -0.555736197296
H 2.292869640594 1.640224166754 0.599937655146
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C 4.430883694125 1.216549342216 -0.807274368653
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C 2.349144342961 0.604549505358 -1.902435336969
H 1.356468483692 0.963258171589 -2.168836374045
H 2.889476424150 0.215474017538 -2.765420804368
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C 3.387950472709 2.746704212187 -2.387799835916
H 2.431129118765 3.113531481619 -2.756218165522
H 3.964110978343 3.570463802658 -1.967715950669
H 3.943288034476 2.280913407007 -3.201180097205
N 3.137585891574 1.739392881390 -1.330798791646

**(C^N^C)Au-Au(C^N^C)**

C -2.659985026336 -0.448750852613 -4.033336491202
C -2.777223324562 -1.820537537352 -4.180456705301
C -2.302288518967 2.561496921212 -3.590525535541

C -2.016101520097 3.876474238984 -3.252056019234
C -1.778416767614 0.085416894993 -3.093295514853
C -2.012545756472 -2.662220331329 -3.384282036323
C -1.638569884032 1.540618422740 -2.913128796238
C -1.091731390332 4.185655187706 -2.264341275988
C -1.132029521637 -2.135361430792 -2.444782247638
C -0.987186982613 -0.763796600264 -2.273257134067
C 5.073313211262 -0.746736205240 -2.182683965085
C -0.444587405045 3.140570481552 -1.608156723988
C 3.774871468603 -0.620074183870 -1.699412870630
C 5.921724649807 -1.719434343485 -1.671690267577
C 0.567234293288 3.221406522653 -0.540767464678
C 3.286285182634 -1.454253921713 -0.700900341519
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C 5.468081129006 -2.565283412022 -0.673723767292
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C 3.661333055860 -3.326889698805 0.879153400832
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C -0.105786257415 -2.161462867858 1.536138140523
C -1.409517275663 -1.710499046871 1.704988575227
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C 1.702352381213 -3.730665192294 2.178284642181
C -2.262825818779 -2.285459230729 2.641381168654
C 0.324977569204 -3.239711317749 2.355591773214
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C 2.343059500462 -4.766080176649 2.855773865196
C -0.535413990212 -3.812550027019 3.292478469184
C -1.827550385957 -3.336438414314 3.437013651472
H -3.262205653109 0.204389018453 -4.656581026804
H -3.463748367555 -2.231263334381 -4.912283537834
H -3.025240984195 2.336731701831 -4.363123771696
H -2.526361020302 4.680649317903 -3.771147944879
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H 6.136578316439 -3.322045123116 -0.276083224450
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H 2.303682475697 5.457633640041 1.330085553756
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H -2.492814434675 -3.784756818819 4.166408784901
Au 0.219685297144 0.352576681075 -0.977240224991
Au 1.420806770618 -1.540723900073 0.245143766651
N -0.756330202095 1.891048038240 -1.970467546703
N 2.396700071588 -3.079202115409 1.238475831886
H 3.132876983288 0.150511685445 -2.110526961779
H -3.275390482826 -1.909857736125 2.749293509057
H -2.102176456671 -3.738273921643 -3.494207959723
H 3.233995760121 3.351853285382 2.244466788188
H 5.424663354988 -0.079858659899 -2.963604132314