Table of content

I. Characterization

General considerations

All manipulations of air-sensitive materials were performed under the rigorous exclusion of oxygen and moisture in flame-dried Schlenk-type glassware either on a dual manifold Schlenk line, interfaced to a high vacuum (10^{-3} torr) line, or in an argon-filled MBraun glove box. Hydrocarbon solvents (toluene & *n*-pentane) were dried by using an MBraun solvent purification system (SPS-800), degassed and stored under vacuo. Tetrahydrofurane was distilled under nitrogen from potassium benzophenone-ketyl before storage over 4 Å molecular sieves. The *n*-butyllithium solution, titanocene dichloride and zirconocene dichloride were purchased from Sigma-Aldrich and were used as received. $[\{HC{\equiv}CC(NDipp)_2\}_2Au_2]$[1, 2] was prepared according to literature.

Nuclear magnetic resonance spectroscopy (NMR)

NMR spectra were recorded on a BrukerAvance II 300 MHz or Avance 400 MHz. Chemical shifts are expressed in parts per million (ppm) and referenced on characteristic solvent resonances as internal standards [7.16 ppm (^{1}H) and 128.06 ppm (^{13}C); thf-d_8: 1.730 ppm (^{1}H) and 25.370 ppm (^{13}C)] and are reported relative to tetramethylsilane. ^{1}H-NMR are reported as follows: chemical shift (δ in ppm), multiplicity (s for singlet, d for doublet, q for quartet, m for multiplet), coupling constant(s) (Hz), number of protons (concluded from the integrals), specific assignment (Ar for aromatic, Ph for phenyl, Cp for cyclopentadienyl, *i* for ipso, *o* for ortho, *m* for meta, *p* for para). ^{13}C{^{1}H} NMR spectra are reported in terms of chemical shift and specific assignment.

Infrared (IR) spectroscopy

IR spectra were obtained on a Bruker Tensor 37 FTIR spectrometer equipped with a room temperature DLaTGS detector, a diamond ATR (attenuated total reflection) unit, and a nitrogen flushed chamber. In terms of their intensity, the signals were classified into the categories vs = very strong, s = strong, m = medium, w = weak and vw = very weak.

Raman spectroscopy

Raman spectra were recorded using a MultiRam spectrometer (Bruker). In terms of their intensity, the signals were classified into the categories vs = very strong, s = strong, m = medium, w = weak and vw = very weak.

Elemental analysis

Elemental analyses were carried out with a Vario Micro Cube (Elementar Analysensysteme GmbH).

Single crystal X-ray diffraction

A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fiber. The crystal was transferred directly to the cold stream of a STOE IPDS 2 or a STOE StadiVari diffractometer. All structures were solved by using the program SHELXS/T[3, 4] and Olex2.[5] The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F^2 by using the program SHELXL.[3] In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance.

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. 2151930-2151931. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

In the structure of compound **1** and **2** some of the (multiple) disordered parts were refined isotropically, since unfavorable overlays in the case of an anisotropic refinement would otherwise have required quite strict restraints & constraints without any additional gain in information.

Photoluminescence measurements

PL measurements were performed with a Horiba Jobin Yvon Fluorolog-322 spectrometer equipped with a closed-cycle optical cryostat (Leybold) operating within a temperature range of 15-300 K. Hamamatsu R9910 and R5509 photomultipliers were used as detectors for the emission spectral ranges of about 300-830 and 500-1380 nm, respectively. The solid samples (crystalline powders) were measured as dispersions in a thin layer of viscous heavy mineral oil (Sigma Aldrich) placed between two 1 mm quartz plates (Material: Spectrosil® 2000). The latter were mounted on the cold finger of the cryostat. All emission spectra were corrected for the wavelength-dependent response of the spectrometer and detector (in relative photon flux units). Emission decay traces were recorded by connecting a photomultiplier to a 500 MHz LeCroy LT322 oscilloscope (via a 50, 500, 2.500 or 10.000 Ohm load depending on the decay time scale) and using a nitrogen laser (~2 nsec, ~5 µJ per pulse) for pulsed excitation at 337 nm. Several hundred traces were usually acquired and averaged. PL

efficiencies of solid complexes at ambient temperature were determined using an integrating sphere out of optical PTFE, which was installed into the sample chamber of the spectrometer, according to the method of de Mello *et al.*[6] The uncertainty of this measurement was estimated to be ±10%.

Quantum chemical calculations

Quantum chemical calculations on Ti_2Au_2 and Zr_2Au_2 complexes **1** and **2** as well as on the structurally related Au_2Au_2 complex - tetranuclear gold(I) bisethinylamidinate $[\{Ph3PAu_2MC{\equiv}CC(NDipp)_2\}_2Au_2]^2$ - were performed with the DFT/TDDFT program package TURBOMOLE[7], using BP86 functional[8-10] as well as Grimme D3 dispersion correction[11] and def-SV(P) basis sets [12]. The optimized geometries of all three complexes were found to possess C_i symmetry. The phosphorescence energies were obtained within the Δ-SCF method for the structure parameters optimized for the triplet state. Table S3 compares the calculated energies with those observed experimentally (for crystalline samples). The theory underestimates the absolute emission energies by about 0.3 eV for **1** and Au_2Au_2 complexes and by 0.5 eV for **2**. Accordingly, however, a trend for the relative energies among these three complexes is reproduced much better, within 0.2 eV.

II. Syntheses

[{ClCp$_2$TiC≡CC(NDipp)$_2$}Au$_2$] (1)

The complex [{HC≡CC(NDipp)$_2$}$_2$Au$_2$] (200 mg, 0.17 mmol, 1.00 eq.) was dissolved in thf (40 mL) and cooled to -78 °C. A 2.5 molar *n*-butyllithium solution in *n*-hexane (144 µL, 0.36 mmol, 2.10 eq.) was added, whereupon the cyan luminescence (observed by irradiation with a conventional UV-Lamp, λ_{exc} = 365nm) of the solution immediately changed color to deep blue. The reaction mixture was stirred for 30 min at -78 °C. Subsequently, titanocene dichloride (85 mg, 0.34 mmol, 2.00 eq.) was added, whereupon the luminescence of the solution immediately vanished. The resulting red solution was warmed to ambient temperature under stirring overnight. The solvent was evaporated and the remaining solid was extracted with 15 mL toluene and was filtered through a syringe filter. After evaporation of the solvent and drying under vacuum the product was obtained as a dark red solid. Red prism shaped single crystals suitable for X-ray analysis were obtained by recrystallization from hot toluene. Yield: 220 mg (81 %)

^{1}H NMR (300 MHz, $CDCl_3$): δ [ppm] = 7.11 (s, 12 H, Ph-*H*), 5.66 (s, 20 H, Cp-*H*), 3.69 (hept, $^3J_{HH}$ = 6.7 Hz, 8 H, C*H*), 1.34 (d, $^3J_{HH}$ = 6.8 Hz, 24 H, CH_3), 1.23 (d, $^3J_{HH}$ = 6.8 Hz, 24 H, CH_3). – **^{13}C{^{1}H}** NMR (75 MHz, $CDCl_3$): δ [ppm] = 159.5 (*C*N$_2$), 154.8 (*C*≡C), 146.0 (*i*-Ph-*C*), 144.2 (*o*-Ph-*C*), 125.6 (*p*-Ph-*C*H), 123.3 (*m*-Ph-*C*H), 120.2 (*C*≡C), 116.2 (Cp-*C*H), 27.8 (*C*H), 24.4 (*C*H$_3$), 24.5 (*C*H$_3$). – **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 2958 (w), 2865 (vw), 2088 (vw), 1484 (vs), 1441 (m), 1369 (m), 1358 (m), 1327 (m), 1319 (m), 1253 (w), 1215 (vw), 1183 (vw), 1100 (vw), 1061 (vw), 1017 (w), 959 (vw), 937 (vw), 826 (vw), 817 (vs), 794 (m), 780 (m), 748 (w), 723 (w), 696 (w), 470 (w), 422 (w). – **Raman** (solid state): $\tilde{\nu}$ [cm^{-1}] = 3130 (vw), 3059 (vw), 2960 (vw), 2933 (vw), 2904 (vw), 2867 (vw), 2088 (vs), 1589 (vw), 1443 (vw), 1369 (w), 1268 (vw), 1133 (w), 450 (vw), 347 (vw), 287 (w), 189 (vw). – **Elemental Analysis**: calcd. (%) for [$C_{74}H_{88}Au_2Cl_2N_4Ti_2$] (1594.11): C 55.76, H 5.56, N 3.51; found: C 56.39, H 5.28, N 3.39.

[{ClCp$_2$ZrC≡CC(NDipp)$_2$}$_2$Au$_2$] (2)

200 mg of **1** (0.17 mmol, 1.00 eq.) were dissolved in 40 mL thf and cooled to -78 °C. A 2.5 molar *n*-butyllithium solution in *n*-hexane (144 µL, 23 mg, 0.36 mmol, 2.10 eq.) was added whereupon the cyan luminescence of the solution immediately changed emission to deep blue. The reaction mixture was stirred for 30 min at -78 °C subsequently a solution of 100 mg of zirconocene dichloride (0.34 mmol, 2.00 eq.) in thf (10 mL) was added, whereupon the luminescence of the solution immediately changed color to yellow. The solution was warmed to ambient temperature under stirring overnight. After evaporation of the solvent the remaining solid was extracted with toluene (20 mL) and was quickly filtered through a thoroughly dried syringe filter. The yellow solution was reduced to approximately 5-10 mL yellow crystals of the title compound were obtained after storage at -30 °C over 3 days. The product was obtained as a yellow solid after decantation of the mother liquor and drying under vacuum. Single crystals suitable for X-ray analysis were grown by layering a concentrated toluene solution with *n*-pentane. Yield: 181 mg (63 %)

^{1}H NMR (400 MHz, C_6D_6): δ [ppm] = 7.13 (s, 12 H, Ph-*H*), 5.46 (s, 20 H, Cp-*H*), 4.06 (hept, $^3J_{HH}$ = 7.0 Hz, 8 H, C*H*), 1.52 (d, $^3J_{HH}$ = 6.9 Hz, 24 H, CH_3), 1.45 (d, $^3J_{HH}$ = 6.8 Hz, 24 H, CH_3). – **^{13}C{^{1}H}** NMR (100 MHz, C_6D_6): δ [ppm] = 160.1 (N*C*N), 149.3 (*C*≡C), 146.3 (*i*-Ph-*C*), 144.4 (*o*-Ph-*C*), 126.3 (*p*-Ph-*C*H), 123.7 (*m*-Ph-*C*H), 115.8 (*C*≡C), 113.2 (Cp-*C*H), 28.3 (*C*H), 24.8 (*C*H$_3$), 24.5 (*C*H$_3$). – **IR** (ATR): $\tilde{\nu}$ [cm^{-1}] = 2958 (m), 2926 (w), 2866 (w), 1485 (s), 1441 (m), 1364 (m), 1322 (m), 1254 (w), 1213 (w), 1179 (w), 1103 (vw), 1059 (vw), 1104 (m), 958 (vw), 937 (vw), 812 (vs), 780 (m), 749 (m), 734 (m), 696 (m), 601 (vw), 538 (vw), 459 (w), 419 (m). – **Raman** (solid state): $\tilde{\nu}$ [cm^{-1}] = 3119 (vw), 3060 (vw), 2963 (w), 2934 (w), 2867 (w), 2094 (vs), 1589 (w), 1445 (w), 1368 (m), 1267 (w), 1180 (vw), 1127 (m), 1003 (vw), 450 (w), 373 (w), 327 (w), 288 (w), 213 (w), 150 (w). – **Elemental Analysis**: calcd. (%) for [$C_{74}H_{88}Au_2Cl_2N_4Zr_2$+0.5 toluene] (1726.90): C 53.90, H 5.37, N 3.24; found: C 54.26, H 5.07, N 3.60.

III. NMR Measurements

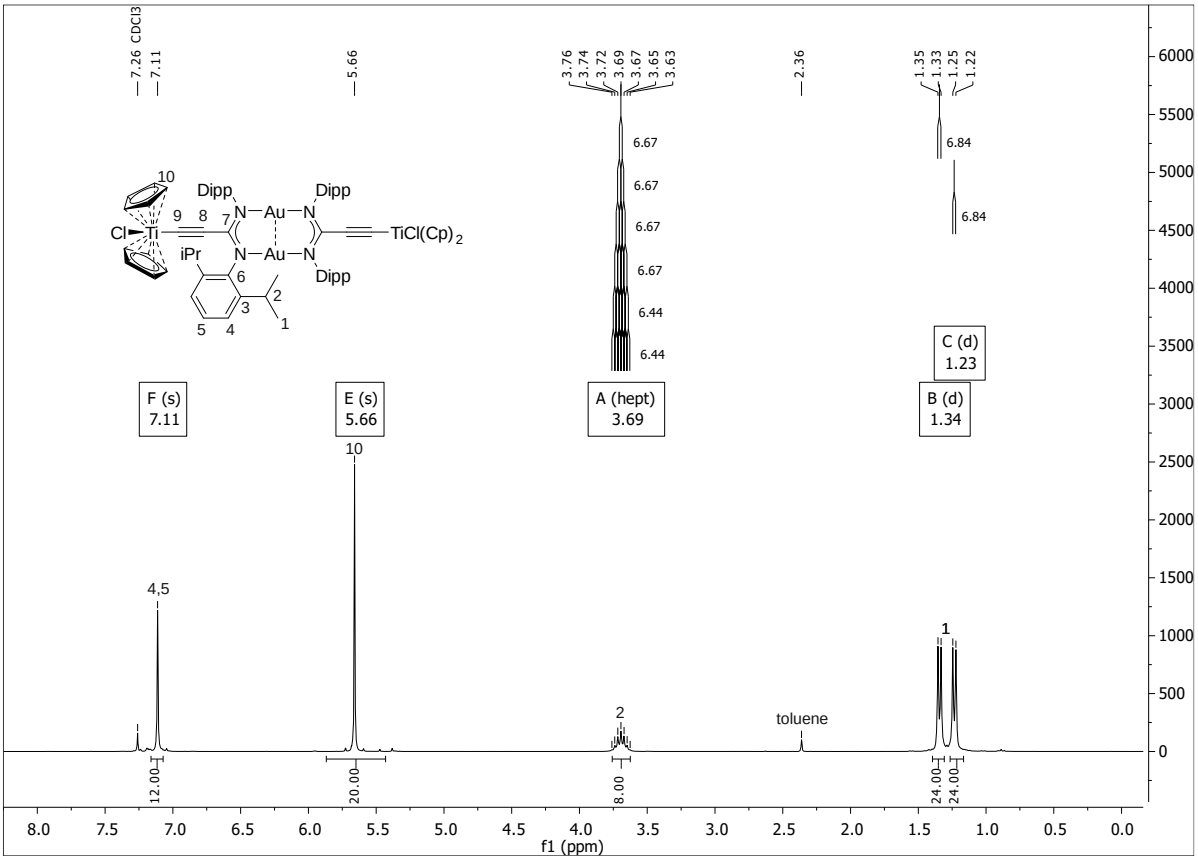

Figure S1 ^{1}H (300 MHz) NMR spectrum of compound **1** in $CDCl_3$ at 25 °C.

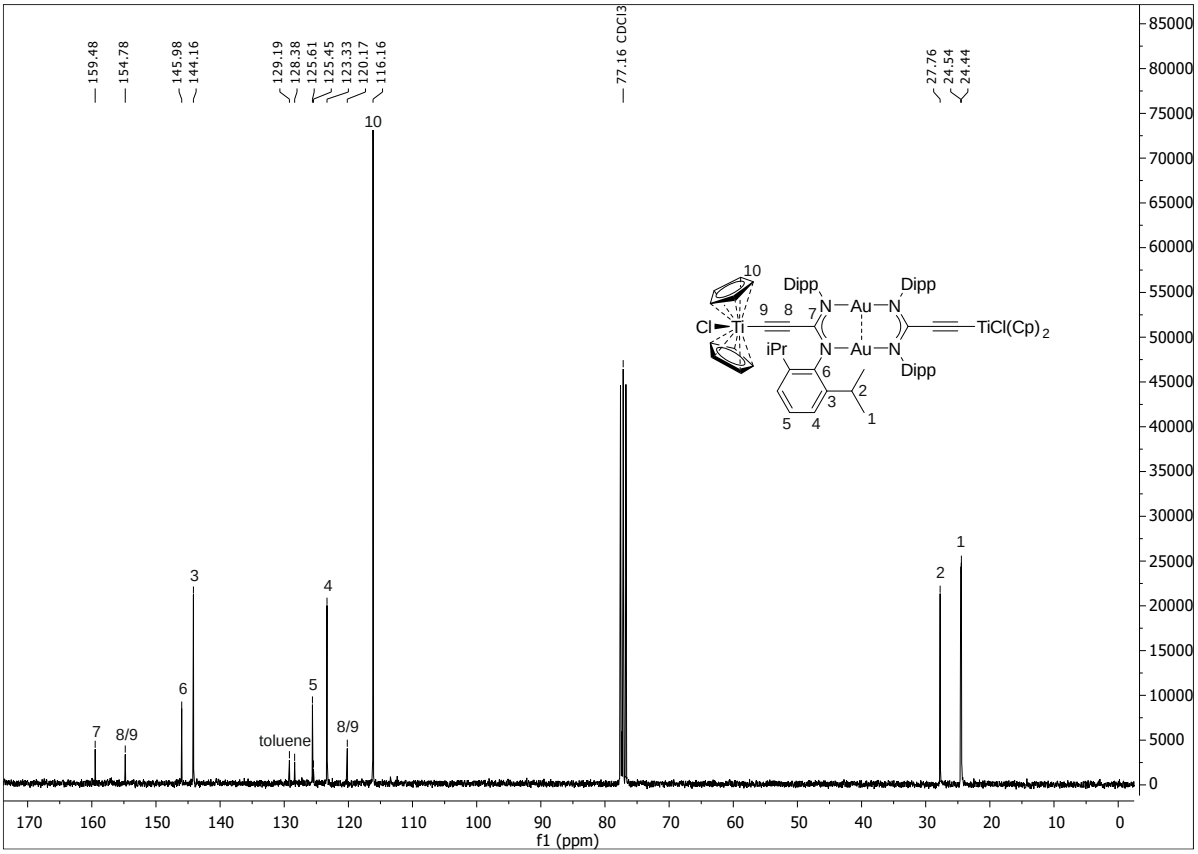

Figure S2 $^{13}C\{^1H\}$ (75 MHz) NMR spectrum of compound **1** in $CDCl_3$ at 25 °C.

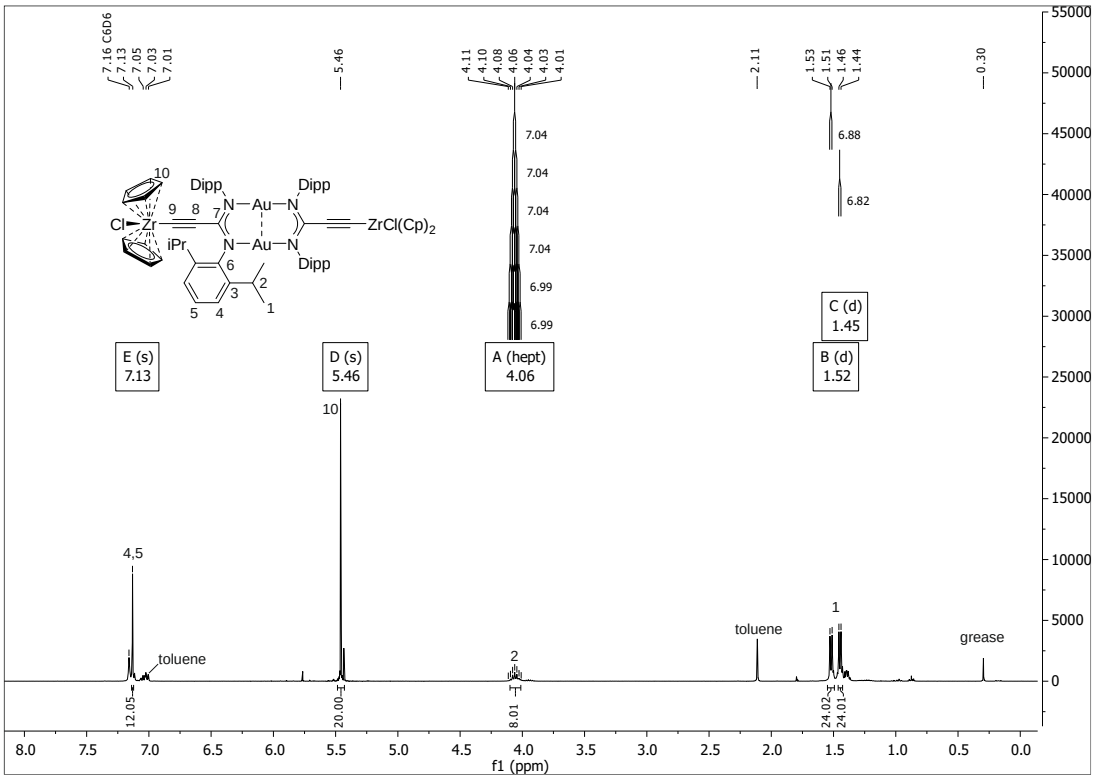

Figure S3 ^1H (400 MHz) NMR spectrum of compound **2** in C_6D_6 at 25 °C.

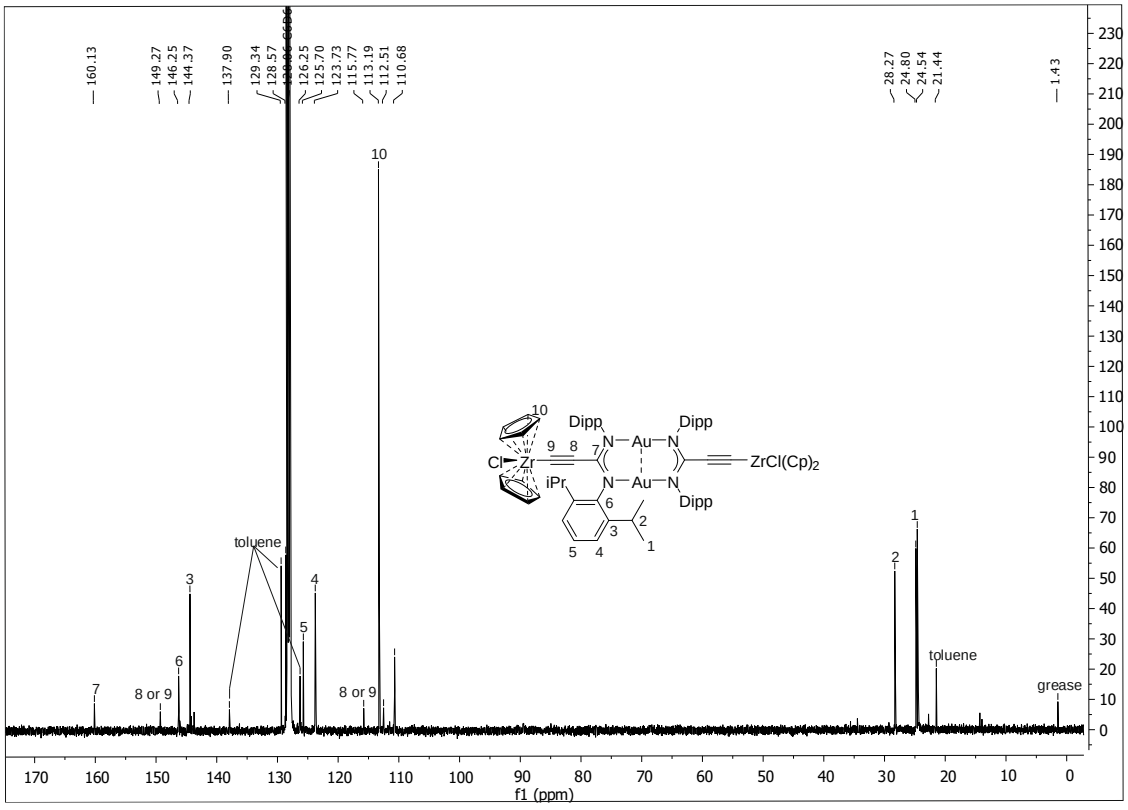

Figure S4 $^{13}C\{^1H\}$ (101 MHz) NMR spectrum of compound **2** in C_6D_6 at 25 °C.

IIII. IR Measurements

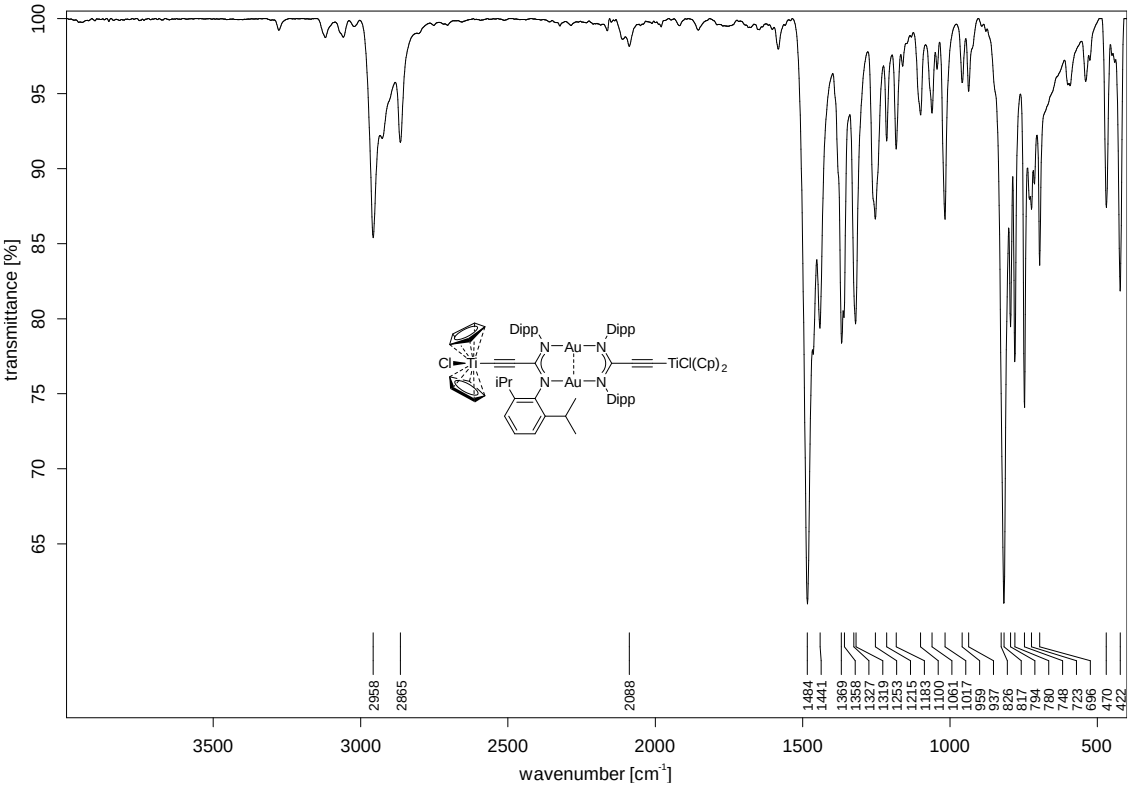

Figure S5: IR (ATR) spectrum of compound **1**.

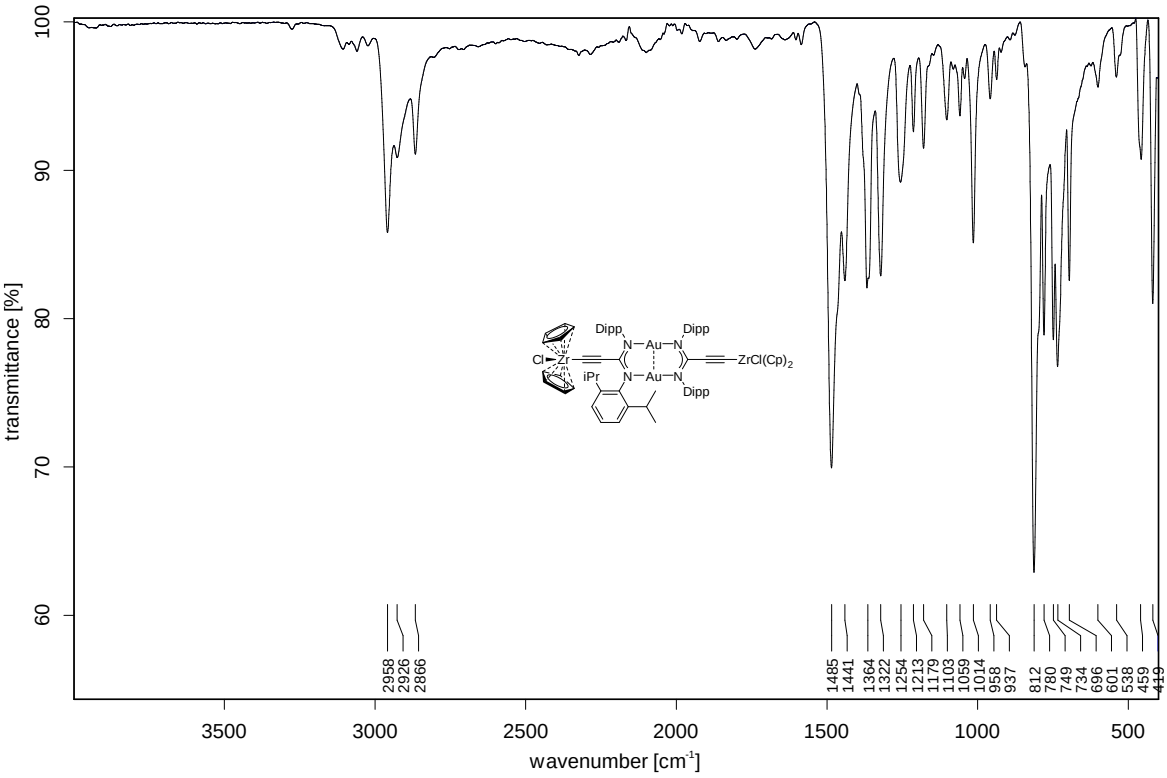

Figure S6: IR (ATR) spectrum of compound **2**.

IV. Raman measurements

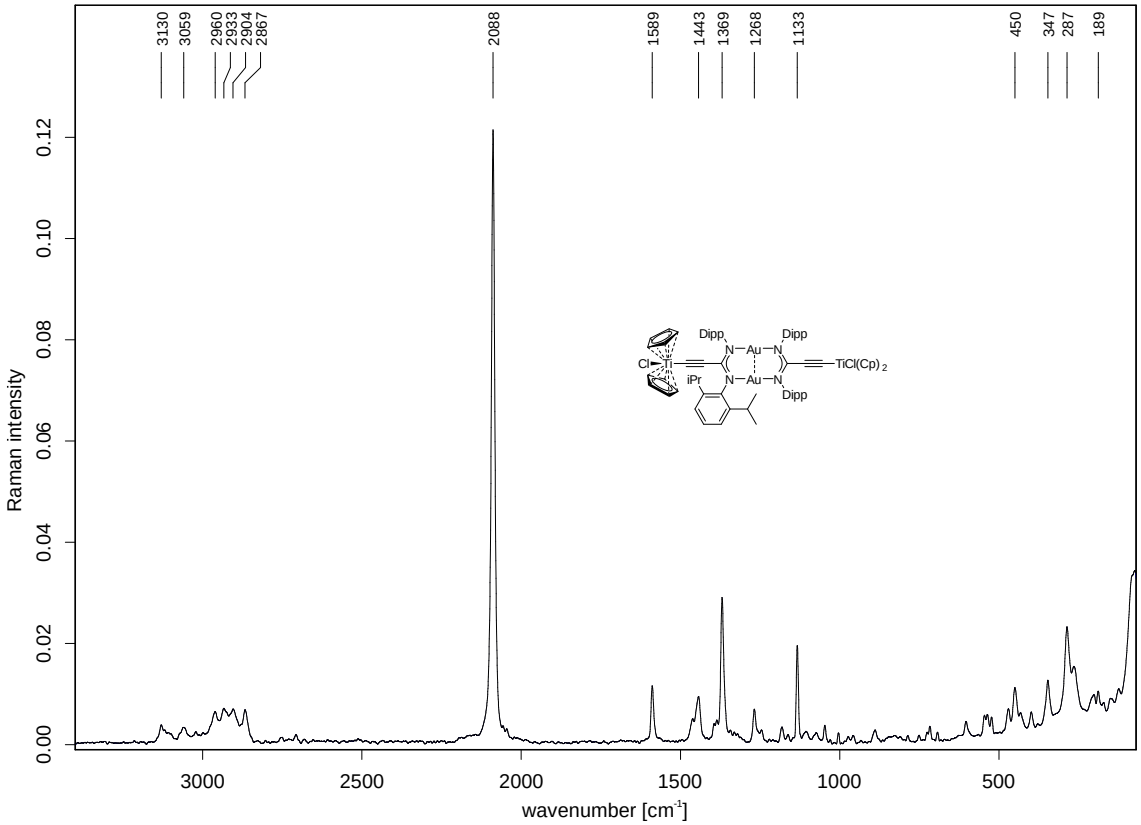

Figure S7 Raman (solid state) spectrum of compound **8**.

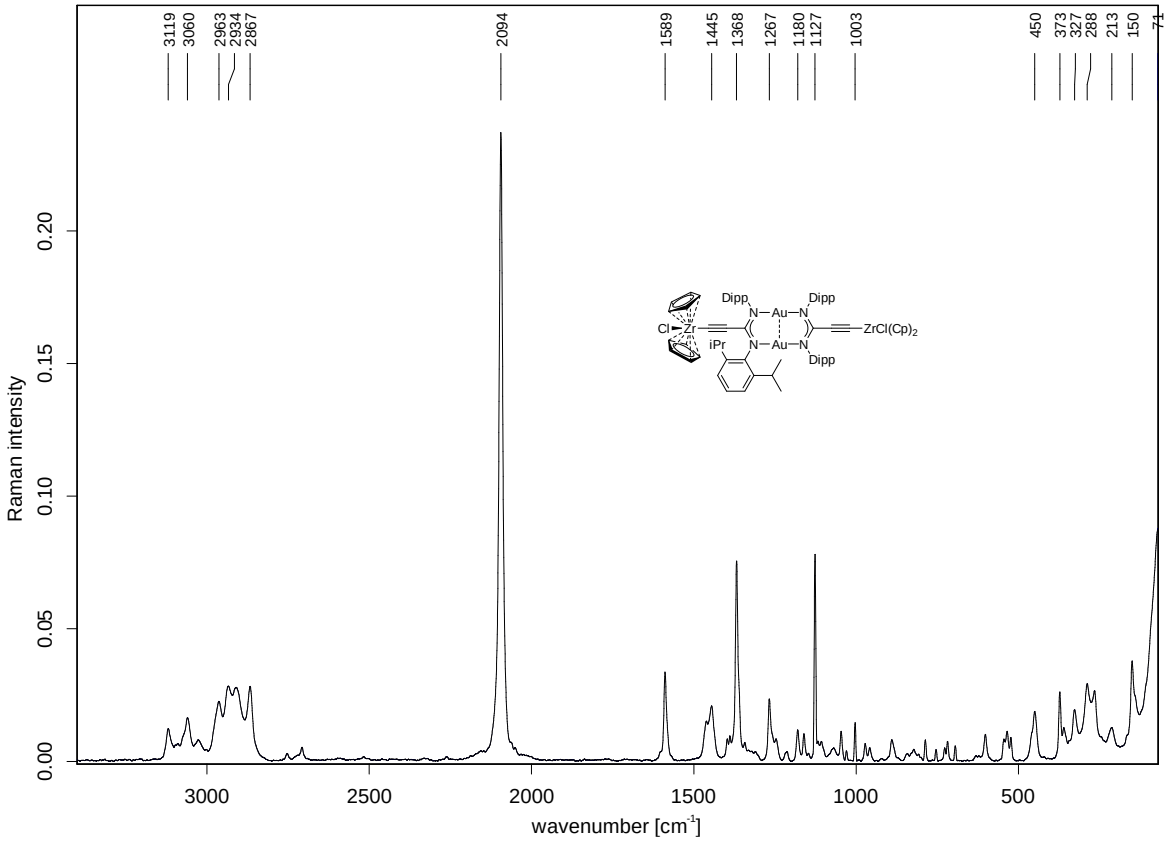

Figure S8 Raman (solid state) spectrum of compound **9**.

VI. Single crystal X-ray diffraction data

Table S1: Crystal data and structure refinement for compounds **1** and **2**.

Compound	**1**·(toluene)$_3$	**2**·(toluene)$_{0.5}$·(pentane)$_{0.25}$
Formula	$C_{95}H_{112}Au_2Cl_2N_4Ti_2$	$C_{83.5}H_{102}Au_2Cl_2N_4Zr_2$
$D_{calc.}$ [g·cm^{-3}]	1.407	1.487
μ [mm^{-1}]	3.593	3.981
Formula Weight	1870.51	1808.96
Colour	red	yellow
Shape	prism-shaped	prism-shaped
Size [mm^3]	0.27×0.17×0.10	0.29×0.16×0.07
T [K]	100	150
Crystal System	triclinic	triclinic
Space Group	$P\bar{1}$	$P\bar{1}$
a [Å]	15.9924(7)	10.2511(4)
b [Å]	16.5310(7)	14.1743(6)
c [Å]	18.2303(8)	14.8080(5)
α [°]	81.979(3)	85.570(3)
β [°]	73.636(4)	73.580(3)
γ [°]	73.059(3)	78.177(3)
V [Å^3]	4415.0(4)	2019.67(14)
Z	2	1
Z'	1	0.5
Wavelength [Å]	0.71073	0.71073
Radiation type	MoK_α	MoK_α
Θ_{min} [°]	1.618	2.031
Θ_{max} [°]	29.659	29.188
Measured Refl.	42976	19024
Independent Refl.	21107	10563
Reflections Used	12501	7514
R_{int}	0.0438	0.0466
Parameters	986	361
Restraints	263	42
Largest Peak	2.227	1.007
Deepest Hole	-1.421	-0.994
GooF	0.942	0.975
wR_2 (all data)	0.1479	0.1087
wR_2	0.1310	0.0982
R_1 (all data)	0.1046	0.0784
R_1	0.0556	0.0457

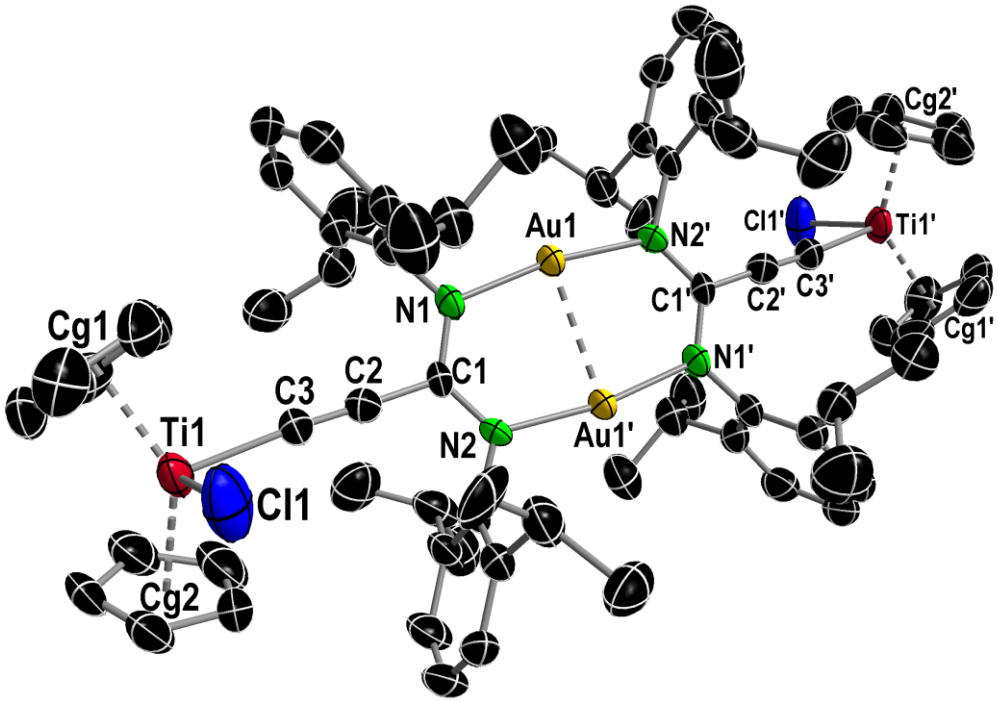

Figure S9 Molecular structure of [{ClCp$_2$TiC≡CC(NDipp)$_2$}Ag]$_2$ (**8**) in the solid state with ellipsoids drawn at 50 % probability. Hydrogen atoms and solvent molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]:

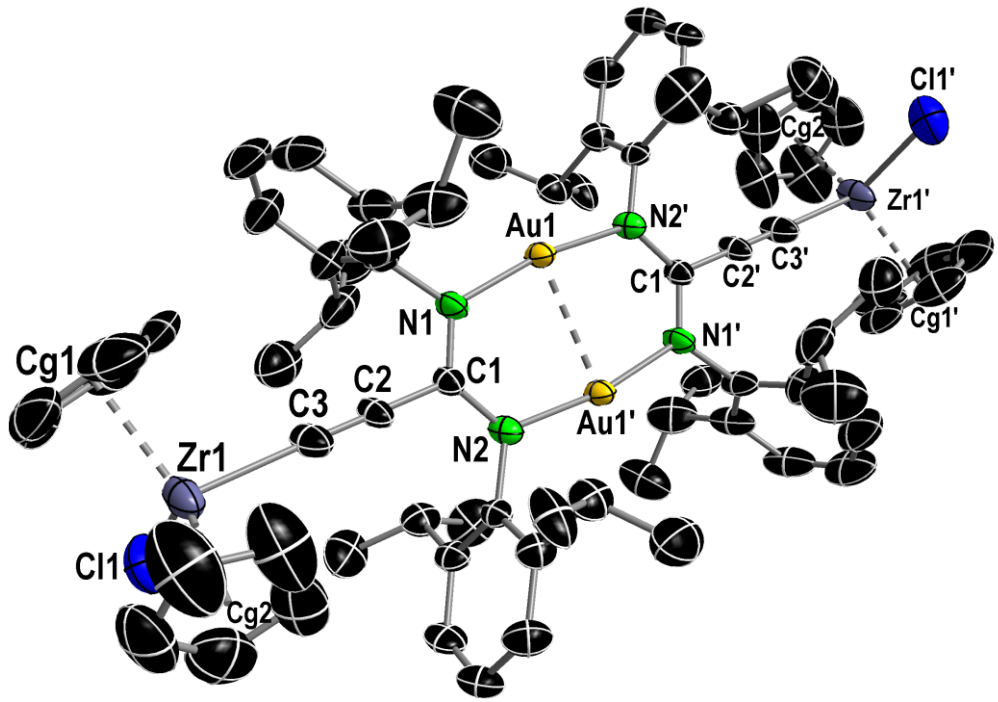

Figure S10 Molecular structure of [{ClCp$_2$ZrC≡CC(NDipp)$_2$}Au]$_2$ (**2**) in the solid state with ellipsoids drawn at 50 % probability. Hydrogen atoms and solvent molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]:

VII. Photoluminescence data

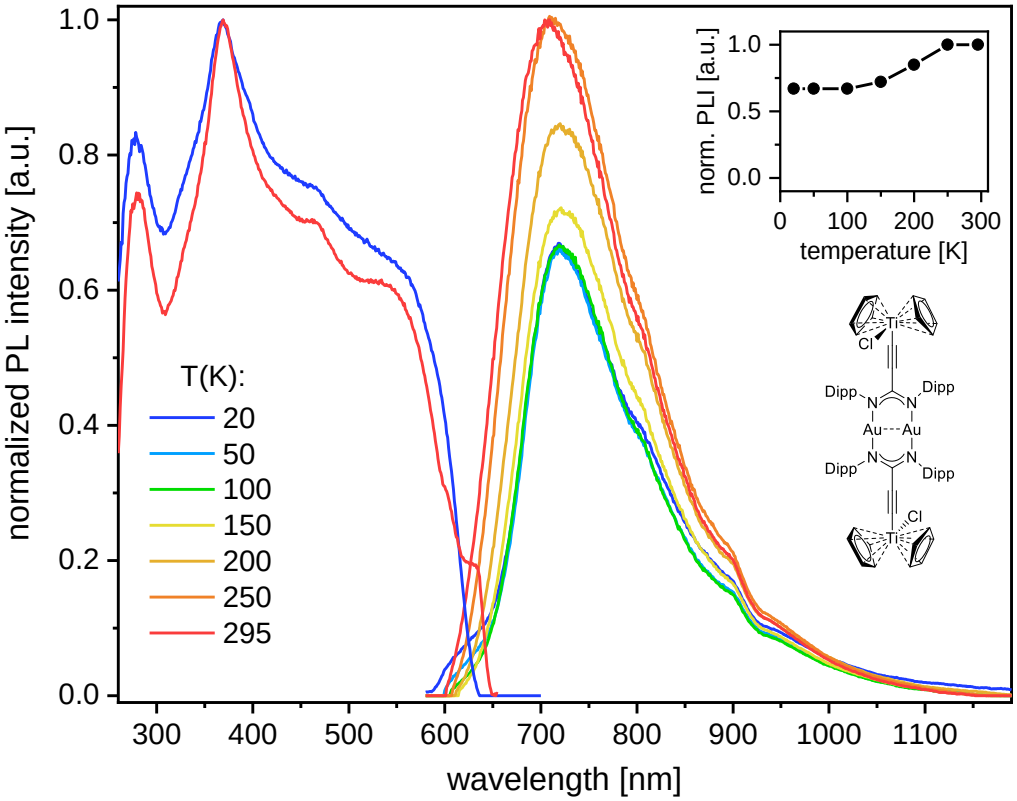

Figure S11 Photoluminescence emission (PL) and excitation (PLE) spectra of polycrystalline compound **1** in the temperature range from 20 to 295 K. The inset depicts the integrated PL intensities versus temperature.

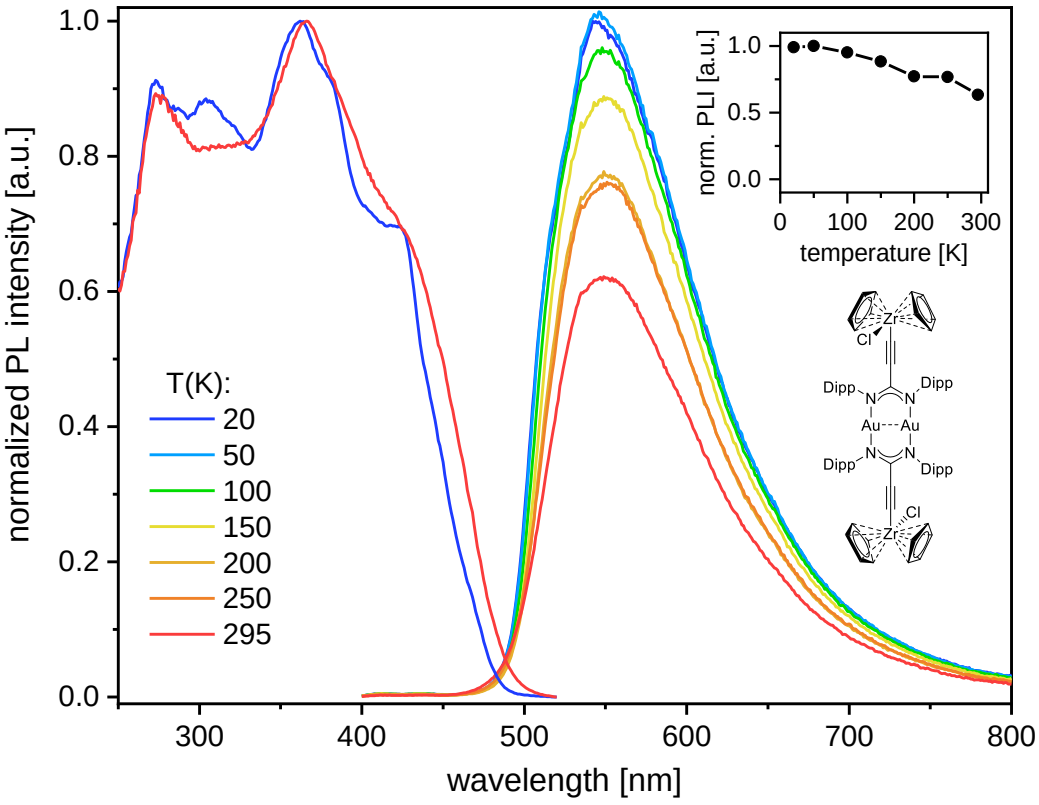

Figure S12 Photoluminescence emission (PL) and excitation (PLE) spectra of polycrystalline compound **2** in the temperature range from 20 to 295 K. The inset depicts the integrated PL intensities versus temperature.

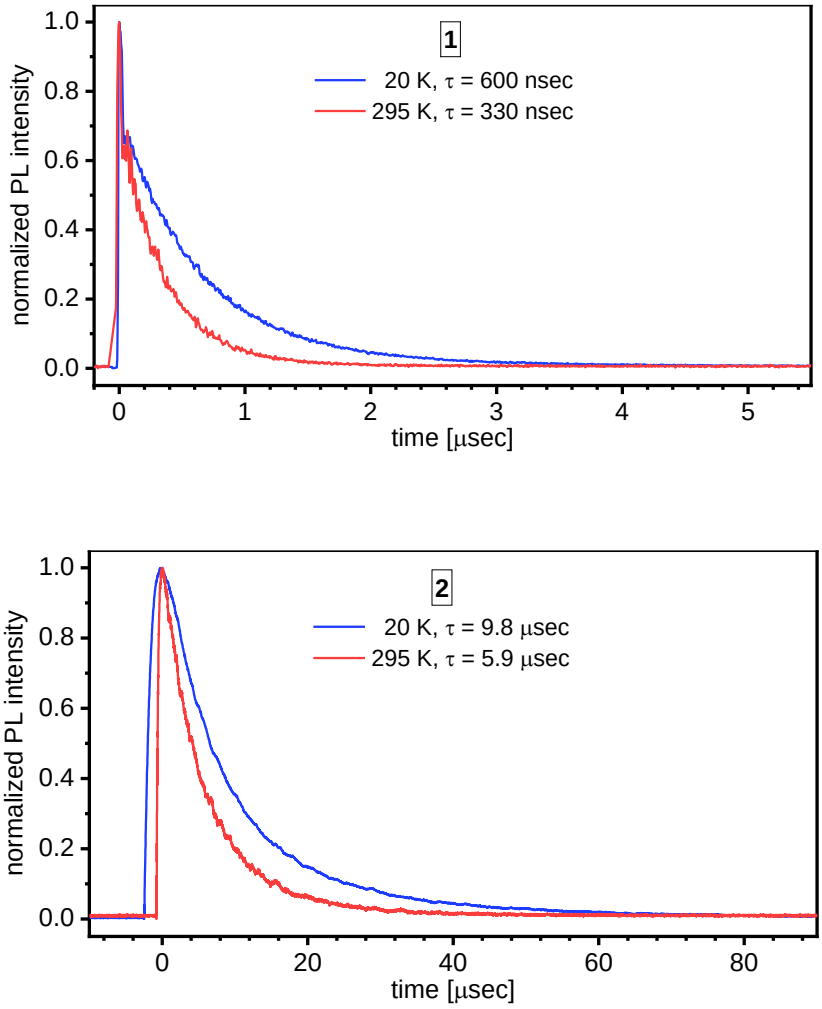

Figure S13 PL decay curves at 20 and 295 K for compound **1** (top) and **2** (bottom).

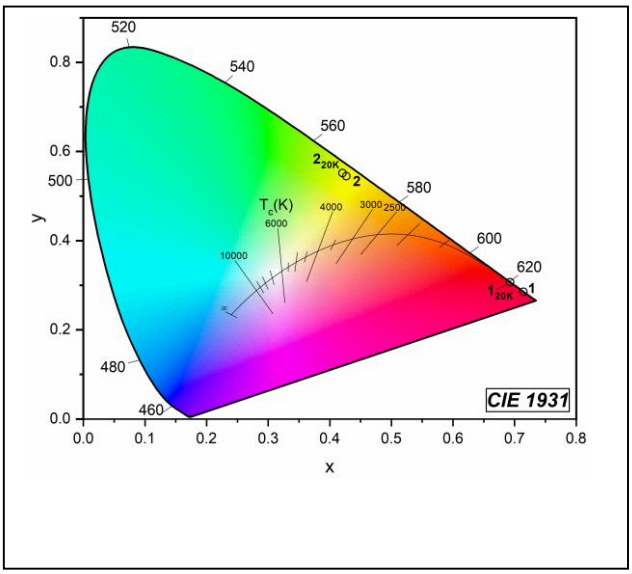

Figure S14 CIE 1931 diagram for compounds 1 and 2 at 295 K and 20 K.

Table S2: Photoluminescence data for compounds **1** and **2**.

Compound		**1**	**2**
Metal atoms		Au_2Ti_2	Au_2Zr_2
λ_{PLE}[a]	[nm]	350	360
λ_{PL}(20/295 K)[b]	[nm]	750 / 710	545 / 550
$\lambda_{PL,Max}$(20 K)[c]	[nm]	720	545
$\lambda_{PL,Max}$(295 K)	[nm]	706	550
FWHM(20 K)[d]	[nm]	147	110
FWHM(295 K)	[nm]	163	108
λ_{PLE}(Φ)[e]	[nm]	450	350
τ(20 K)[f]	[µs]	0.60	9.8
τ(295 K)	[µs]	0.33	5.9
Φ(RT)[g]	[%]	0.6	41

[a] excitation wavelength for the measurement of the PL spectra. [b] emission wavelength for the measurement of the PLE spectra at 20 and 295 K, respectively. [c] emission maxima. [d] full width at half maximum of the emission bands. [e] excitation wavelength for the quantum yield determination. [f] PL lifetimes determined via monoexponential fits of the measured PL decay curves. [g] PL quantum yield at ambient temperature.

Table S3: DFT/Δ-SCF calculated and experimentally observed phosphorescence energies of tetranuclear Ti_2Au_2 (**1**) and Zr_2Au_2 (**2**) described in this work and related Au_2Au_2 complex $[\{Ph_3PAu_2MC{\equiv}CC(NDipp)_2\}_2Au_2]$ (M = Ti, Zr and Au, respectively).[2]

M	Au	Ti	Zr
E_{tot} (Singlet Ground state)/ a.u.	-4931.50342	-5981.17795	-4376.495053
E_{tot} (Triplet state)/ a.u.	-4931.41370	-5981.12322	-4376.424045
E_{tot} (Singlet of Triplet state geometry)/ a.u.	-4931.49712	-5981.17344	-4376.489406
calc.:			
ΔE/ eV	2.27	1.37	1.78
λ/ nm	546.2	907.3	697.1
exp.:			
ΔE/ eV	2.58/2.61[a]	1.72/1.76	2.27/2.25
λ/ nm (20/ 295 K)	480/475[a]	720/706	545/550

[a] approx. center energy/ wavelength of vibronically structured phosphorescence band (Ref. 1).

VIII. UV-Vis Spectra

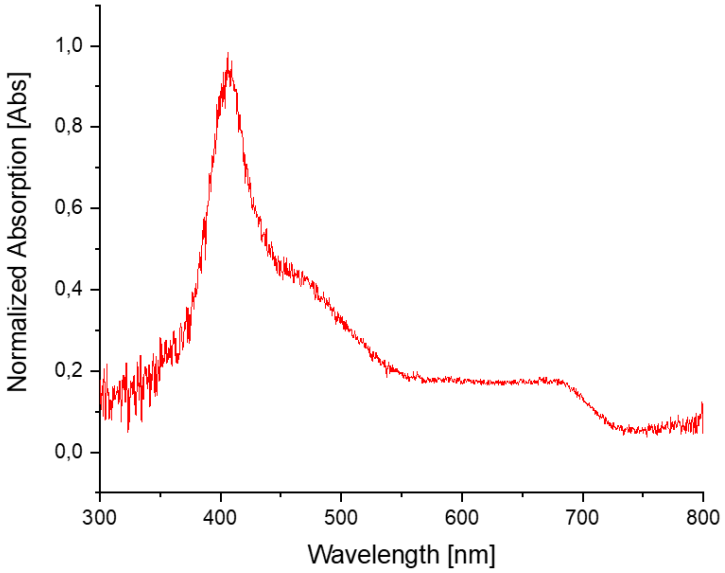

Figure S15 UV-Vis spectrum of compound **1** in THF.

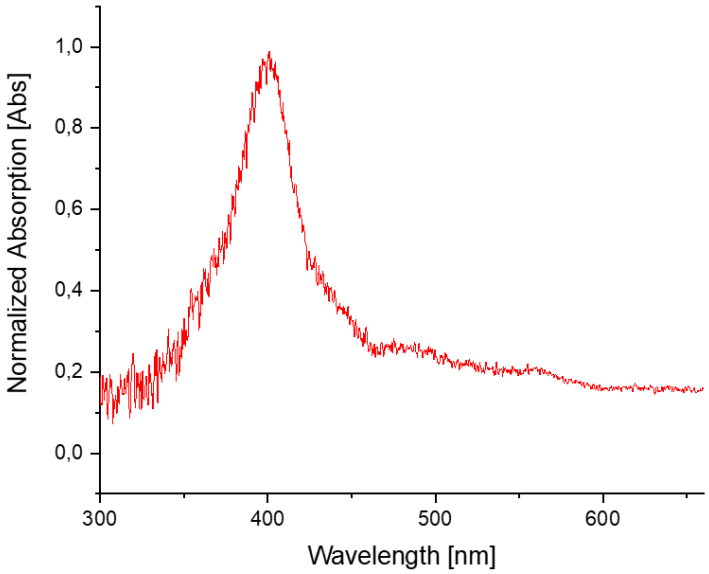

Figure S16 UV-Vis spectrum of compound **2** in THF.

IX. Quantum Chemical Calculations

Cartesian Coordinates of the molecules under discussion

[{ClCp$_2$TiC≡CC(NDipp)$_2$}$_2$Au$_2$] **1** (singlet ground state)

-13.97850585125257	0.01627973507683	-0.59837875916837	ti
-16.70533571207911	-3.47595175841357	-1.50453958678117	c
-16.74857956804646	-3.07403345574539	1.15440167892205	c
-14.26731103622407	-3.55408599325974	2.10832396844140	c
-12.71238292853305	-4.33163666386119	0.04468760817417	c
-14.20877734924857	-4.25665911214226	-2.18341093011939	c
-18.28324079608695	-3.16666384369322	-2.81729022442314	h
-18.39110595649781	-2.47804398634047	2.27181178034304	h
-13.65521659111364	-3.40250635772681	4.08486672995993	h
-10.71730871074826	-4.87226227670772	0.15309396028724	h
-13.52457155042958	-4.64434449146128	-4.09875847152903	h
-0.01931803349302	-2.62769246220761	0.10449692178107	au
-3.89266478105045	-2.20507278090497	0.07244772201542	n
-5.06930367472616	0.05523438271251	-0.06099817968702	c
-7.76370885351829	0.03431441700872	-0.21820239752443	c
-10.09873150875273	-0.02532031869447	-0.39221735703773	c
-7.24397256456846	-8.11944770928022	1.96356049862529	c
-5.99393605911826	-5.77769738140248	2.16843172761826	c
-5.34559469181245	-4.47957872104255	-0.08842223662750	c
-5.97046098395383	-5.46657461558545	-2.50447893671529	c
-7.24623874609307	-7.80153547355401	-2.61702139120940	c
-7.86236172689660	-9.13506965280528	-0.40790626442029	c
-7.76567085984225	-9.15387004900770	3.69491497140420	h
-7.76331400333179	-8.59920709270796	-4.47279492429966	h
-8.85679403653210	-10.96117512624353	-0.53621824374064	h
-5.44242842746602	-4.59588776235198	4.73766784173705	c
-7.90963158981266	-3.59908482034642	5.93867566746996	c
-9.22498753132555	-5.18222056126814	6.38220150782410	h
-7.50047279570603	-2.56908330285135	7.72776805027761	h
-8.89979524813029	-2.28554127007056	4.63053969842395	h
-4.00919365576964	-6.39030801410716	6.52512898805495	c
-4.20297513499193	-2.93600675579278	4.39194977268528	h
-3.50074426496387	-5.39871504340521	8.30859575982379	h
-2.22978289683589	-7.06910010639792	5.63679566229460	h
-5.16271639705211	-8.07393855892236	7.04172650502787	h
-5.24108929737679	-4.05624952846303	-4.90793390125272	c
-3.20405952831726	-5.51723952925488	-6.39449102398901	c
-7.57543394315630	-3.40991946305704	-6.52191237301613	c
-3.92220003091375	-7.36350544888784	-7.10169847709536	h
-8.54899902678461	-5.15117757492317	-7.19681479320456	h
-2.54099832077065	-4.39937926961165	-8.04965703583331	h
-7.02205272124577	-2.30458003713842	-8.22367109170747	h
-1.53901260285851	-5.89881178867479	-5.16896427970765	h
-8.95919037956241	-2.26257471233557	-5.42977312708346	h
-4.35910506065933	-2.24371890517267	-4.32932014917719	h
13.97850585125257	-0.01627973507683	0.59837875916837	ti
15.73498739238163	-4.22914904180321	0.54441491605438	c
-17.02291617091603	2.70300758732310	1.26581712505998	c
16.74857956804646	3.07403345574539	-1.15440167892205	c
-15.73498739238163	4.22914904180321	-0.54441491605438	c
16.70533571207911	3.47595175841357	1.50453958678117	c

17.02291617091603	-2.70300758732310	-1.26581712505998	c
15.24743189273238	-2.06701301394771	-3.21258469635106	c
-13.16891664122984	4.44426514236201	0.20554364109815	c
14.20877734924857	4.25665911214226	2.18341093011939	c
-15.24743189273238	2.06701301394771	3.21258469635106	c
14.26731103622407	3.55408599325974	-2.10832396844140	c
13.16891664122984	-4.44426514236201	-0.20554364109815	c
12.87628973960333	-3.12260930076539	-2.54884183434621	c
-12.87628973960333	3.12260930076539	2.54884183434621	c
12.71238292853305	4.33163666386119	-0.04468760817417	c
16.54978276043484	-4.98614263787841	2.29214808318108	h
-19.03126967739895	2.18380133820694	1.21452127012776	h
18.39110595649781	2.47804398634047	-2.27181178034304	h
-16.54978276043484	4.98614263787841	-2.29214808318108	h
18.28324079608695	3.16666384369322	2.81729022442314	h
19.03126967739895	-2.18380133820694	-1.21452127012776	h
15.64102530312888	-0.94399983715461	-4.91193826231995	h
-11.64006654454949	5.37469046143544	-0.84459050283415	h
13.52457155042958	4.64434449146128	4.09875847152903	h
-15.64102530312888	0.94399983715461	4.91193826231995	h
13.65521659111364	3.40250635772681	-4.08486672995993	h
11.64006654454949	-5.37469046143544	0.84459050283415	h
11.11529809533681	-2.94926975793972	-3.61986286560408	h
-11.11529809533681	2.94926975793972	3.61986286560408	h
10.71730871074826	4.87226227670772	-0.15309396028724	h
0.01931803349302	2.62769246220761	-0.10449692178107	au
3.87999289293300	-2.31364663763574	0.07300687113836	n
-3.87999289293300	2.31364663763574	-0.07300687113836	n
3.89266478105045	2.20507278090497	-0.07244772201542	n
5.06930367472616	-0.05523438271251	0.06099817968702	c
7.76370885351829	-0.03431441700872	0.21820239752443	c
10.09873150875273	0.02532031869447	0.39221735703773	c
7.06006393374211	-8.35504470258976	-1.67580782916367	c
-7.64764611755567	7.61957391012921	-2.81927114202983	c
7.24623874609307	7.80153547355401	2.61702139120940	c
-7.06006393374211	8.35504470258976	1.67580782916367	c
7.24397256456846	8.11944770928022	-1.96356049862529	c
7.64764611755567	-7.61957391012921	2.81927114202983	c
5.67920441528265	-6.09162505371701	-1.91528440595137	c
-6.29081961040273	5.33421485505331	-2.67920946321590	c
5.97046098395383	5.46657461558545	2.50447893671529	c
-5.67920441528265	6.09162505371701	1.91528440595137	c
5.99393605911826	5.77769738140248	-2.16843172761826	c
6.29081961040273	-5.33421485505331	2.67920946321590	c
5.34325283742626	-4.57865084585436	0.27881849971109	c
-5.34325283742626	4.57865084585436	-0.27881849971109	c
5.34559469181245	4.47957872104255	0.08842223662750	c
8.04692881630570	-9.11248407058276	0.66459696589663	c
-8.04692881630570	9.11248407058276	-0.66459696589663	c
7.86236172689660	9.13506965280528	0.40790626442029	c
7.36536024654314	-9.55779340384312	-3.34647508100439	h
-8.41475684116472	8.24265580844133	-4.65091603605995	h
7.76331400333179	8.59920709270796	4.47279492429966	h
-7.36536024654314	9.55779340384312	3.34647508100439	h
7.76567085984225	9.15387004900770	-3.69491497140420	h
8.41475684116472	-8.24265580844133	4.65091603605995	h
9.13414808001315	-10.88464661302431	0.81124289499757	h
-9.13414808001315	10.88464661302431	-0.81124289499757	h
8.85679403653210	10.96117512624353	0.53621824374064	h

4.55211786838246	-5.24971723791902	-4.43581732167585	c
-5.74048894902024	3.77580876648465	-5.04292875535723	c
5.24108929737679	4.05624952846303	4.90793390125272	c
-4.55211786838246	5.24971723791902	4.43581732167585	c
5.44242842746602	4.59588776235198	-4.73766784173705	c
5.74048894902024	-3.77580876648465	5.04292875535723	c
6.27644290374070	-3.31438470249790	-5.76538742455885	c
-7.88269187150653	3.82997101250979	-7.00048567191777	c
7.57543394315630	3.40991946305704	6.52191237301613	c
-6.27644290374070	3.31438470249790	5.76538742455885	c
7.90963158981266	3.59908482034642	-5.93867566746996	c
7.88269187150653	-3.82997101250979	7.00048567191777	c
8.07360114348081	-4.22675248128382	-6.37418109999551	h
-8.06187716388843	5.71443085160418	-7.91779764737806	h
8.54899902678461	5.15117757492317	7.19681479320456	h
-8.07360114348081	4.22675248128382	6.37418109999551	h
9.22498753132555	5.18222056126814	-6.38220150782410	h
8.06187716388843	-5.71443085160418	7.91779764737806	h
5.34165360814067	-2.52727733560311	-7.47942914386907	h
-7.48635319288220	2.44127487166033	-8.52677635792585	h
7.02205272124577	2.30458003713842	8.22367109170747	h
-5.34165360814067	2.52727733560311	7.47942914386907	h
7.50047279570603	2.56908330285135	-7.72776805027761	h
7.48635319288220	-2.44127487166033	8.52677635792585	h
6.76207876807861	-1.71381752194565	-4.50073882685032	h
-9.72946222504516	3.31950473732033	-6.13556106905414	h
8.95919037956241	2.26257471233557	5.42977312708346	h
-6.76207876807861	1.71381752194565	4.50073882685032	h
8.89979524813029	2.28554127007056	-4.63053969842395	h
9.72946222504516	-3.31950473732033	6.13556106905414	h
3.88919188114586	-7.44563273433013	-6.22207638535941	c
-3.19273180316554	4.59987931489233	-6.20966389179882	c
3.20405952831726	5.51723952925488	6.39449102398901	c
-3.88919188114586	7.44563273433013	6.22207638535941	c
4.00919365576964	6.39030801410716	-6.52512898805495	c
3.19273180316554	-4.59987931489233	6.20966389179882	c
2.75274896300057	-4.25256108193018	-3.98917465021158	h
-5.51915463527177	1.77838621689279	-4.44785545873222	h
4.35910506065933	2.24371890517267	4.32932014917719	h
-2.75274896300057	4.25256108193018	3.98917465021158	h
4.20297513499193	2.93600675579278	-4.39194977268528	h
5.51915463527177	-1.77838621689279	4.44785545873222	h
2.78838276451984	-6.73224527761459	-7.86322070360887	h
-2.72604997690092	3.41873821605022	-7.88644034788572	h
2.54099832077065	4.39937926961165	8.04965703583331	h
-2.78838276451984	6.73224527761459	7.86322070360887	h
3.50074426496387	5.39871504340521	-8.30859575982379	h
2.72604997690092	-3.41873821605022	7.88644034788572	h
2.73024734347516	-8.90132261791960	-5.24437834515363	h
-1.62269080252341	4.38967173285052	-4.82373602398954	h
1.53901260285851	5.89881178867479	5.16896427970765	h
-2.73024734347516	8.90132261791960	5.24437834515363	h
2.22978289683589	7.06910010639792	-5.63679566229460	h
1.62269080252341	-4.38967173285052	4.82373602398954	h
5.60786024745858	-8.38254392527798	-6.99371684709516	h
-3.25260507842533	6.61391463404196	-6.82030257362511	h
3.92220003091375	7.36350544888784	7.10169847709536	h
-5.60786024745858	8.38254392527798	6.99371684709516	h
5.16271639705211	8.07393855892236	-7.04172650502787	h

3.25260507842533	-6.61391463404196	6.82030257362511	h
14.15113618597437	-0.84776463449982	4.90130296952760	cl
-14.15113618597437	0.84776463449982	-4.90130296952760	cl

[{ClCp$_2$TiC≡CC(NDipp)$_2$}$_2$Au$_2$] **1** (triplet state)

-13.99530351264388	-0.06095569740582	-0.64536803858081	ti
-16.66536488059442	-3.66344969572200	-1.10077624143252	c
-16.81302670621230	-2.85898286852832	1.46712429370047	c
-14.37769973704578	-3.18198062404818	2.58857014599946	c
-12.74794123292800	-4.25952599880404	0.72792999629323	c
-14.14907367955649	-4.54034587050991	-1.54371410171611	c
-18.19014131401935	-3.58118945031983	-2.50560707934817	h
-18.49901410265262	-2.10946604389975	2.41376769991411	h
-13.84017659277488	-2.70514314451163	4.53492421482644	h
-10.75845453999309	-4.76514144344394	0.99222489585800	h
-13.38723320526914	-5.20729050552439	-3.35051354977365	h
-0.02097223894766	-2.58917538384502	0.05446861417947	au
-3.86669542471121	-2.21985388573253	0.21571083581360	n
-5.09537943771346	0.04240952172514	0.07549464243032	c
-7.75285646534395	0.04472466969360	-0.11946434140992	c
-10.09823083826120	-0.02165293222597	-0.34419785004039	c
-7.14871978269709	-8.19900946539357	1.98048304976666	c
-5.86168956735060	-5.88465485019388	2.23476447492527	c
-5.32209861640186	-4.49182275221268	0.00512097391187	c
-6.07345217765422	-5.35101831520508	-2.42770043529429	c
-7.35751582563408	-7.67416380326983	-2.57874683315018	c
-7.88517759186236	-9.09625176019981	-0.40323196002203	c
-7.62301019788301	-9.30051153109880	3.68296671660456	h
-7.94721976934286	-8.39400477300840	-4.44170248098954	h
-8.90101017201781	-10.90739045079477	-0.56462263798383	h
-5.26508936473195	-4.78515797763975	4.82763136180781	c
-7.70861597603231	-3.69422721478108	5.99957184092069	c
-9.09555830504841	-5.22893974889002	6.38840461550196	h
-7.29633083787534	-2.70580724328464	7.81007404480842	h
-8.61902595581788	-2.32862664452599	4.68806138489106	h
-3.95960183656471	-6.68093911179509	6.60514734505671	c
-3.94194103028989	-3.17990294327289	4.53465759353254	h
-3.38518729746540	-5.73237102664844	8.39159961844077	h
-2.23429723121065	-7.48656445571194	5.71727848547829	h
-5.22835077588340	-8.27654499371326	7.12378722156705	h
-5.38024080104277	-3.88328626564364	-4.80635891300564	c
-3.10755772927470	-5.14710474970132	-6.12901521662124	c
-7.64034881159557	-3.50015431981795	-6.59374628048872	c
-3.59208492151218	-7.08724266476860	-6.78074251017886	h
-8.34043623379443	-5.32026320313377	-7.38351367489691	h
-2.49856719413891	-4.02760264814478	-7.80275438600242	h
-7.07312180844321	-2.29582985255632	-8.22069066583886	h
-1.46596942572889	-5.30157035899294	-4.82113573326358	h
-9.23752898706653	-2.54651856655314	-5.61668599254945	h
-4.74405471134238	-1.97387406670576	-4.21514404317184	h
13.99530351264388	0.06095569740582	0.64536803858081	ti
15.93454439420685	-3.97739210323994	1.48415868765594	c
-17.22221721860712	2.84807916409105	0.58840611683202	c
16.81302670621230	2.85898286852832	-1.46712429370047	c
-15.93454439420685	3.97739210323994	-1.48415868765594	c
16.66536488059442	3.66344969572200	1.10077624143252	c
17.22221721860712	-2.84807916409105	-0.58840611683202	c

15.47749066429896	-2.66769748616579	-2.65527214763052	c
-13.39032353631635	4.43275825998628	-0.73809171219515	c
14.14907367955649	4.54034587050991	1.54371410171611	c
-15.47749066429896	2.66769748616579	2.65527214763052	c
14.37769973704578	3.18198062404818	-2.58857014599946	c
13.39032353631635	-4.43275825998628	0.73809171219515	c
13.11716815280192	-3.64619933306601	-1.83625388217068	c
-13.11716815280192	3.64619933306601	1.83625388217068	c
12.74794123292800	4.25952599880404	-0.72792999629323	c
16.72050985542547	-4.30958950249597	3.37208155280267	h
-19.20923684033113	2.25170495190307	0.60612069903379	h
18.49901410265262	2.10946604389975	-2.41376769991411	h
-16.72050985542547	4.30958950249597	-3.37208155280267	h
18.19014131401935	3.58118945031983	2.50560707934817	h
19.20923684033113	-2.25170495190307	-0.60612069903379	h
15.89038818219218	-1.88665790989176	-4.53236119841058	h
-11.86492129812239	5.17956951396789	-1.92553724947643	h
13.38723320526914	5.20729050552439	3.35051354977365	h
-15.89038818219218	1.88665790989176	4.53236119841058	h
13.84017659277488	2.70514314451163	-4.53492421482644	h
11.86492129812239	-5.17956951396789	1.92553724947643	h
11.37082203246217	-3.75979962410985	-2.94507599112887	h
-11.37082203246217	3.75979962410985	2.94507599112887	h
10.75845453999309	4.76514144344394	-0.99222489585800	h
0.02097223894766	2.58917538384502	-0.05446861417947	au
3.83556076057866	-2.29152148986180	-0.14805309898365	n
-3.83556076057866	2.29152148986180	0.14805309898365	n
3.86669542471121	2.21985388573253	-0.21571083581360	n
5.09537943771346	-0.04240952172514	-0.07549464243032	c
7.75285646534395	-0.04472466969360	0.11946434140992	c
10.09823083826120	0.02165293222597	0.34419785004039	c
7.02066834909123	-8.28656369971118	-1.99757935706162	c
-7.53191177637399	7.66949544746982	-2.52912091873721	c
7.35751582563408	7.67416380326983	2.57874683315018	c
-7.02066834909123	8.28656369971118	1.99757935706162	c
7.14871978269709	8.19900946539357	-1.98048304976666	c
7.53191177637399	-7.66949544746982	2.52912091873721	c
5.63744843782423	-6.02517706085058	-2.19963600557441	c
-6.20345193581091	5.36969501585243	-2.42682942262593	c
6.07345217765422	5.35101831520508	2.42770043529429	c
-5.63744843782423	6.02517706085058	2.19963600557441	c
5.86168956735060	5.88465485019388	-2.23476447492527	c
6.20345193581091	-5.36969501585243	2.42682942262593	c
5.27757274090501	-4.57019053594938	0.03134828090180	c
-5.27757274090501	4.57019053594938	-0.03134828090180	c
5.32209861640186	4.49182275221268	-0.00512097391187	c
7.96056738099568	-9.10644933630409	0.34187814217088	c
-7.96056738099568	9.10644933630409	-0.34187814217088	c
7.88517759186236	9.09625176019981	0.40323196002203	c
7.37328483879585	-9.43265940700328	-3.69872206069749	h
-8.25653819617341	8.35173239594273	-4.35744108423187	h
7.94721976934286	8.39400477300840	4.44170248098954	h
-7.37328483879585	9.43265940700328	3.69872206069749	h
7.62301019788301	9.30051153109880	-3.68296671660456	h
8.25653819617341	-8.35173239594273	4.35744108423187	h
9.03492240013417	-10.88697952976274	0.46308676157905	h
-9.03492240013417	10.88697952976274	-0.46308676157905	h
8.90101017201781	10.90739045079477	0.56462263798383	h
4.68040129548146	-5.05461078052645	-4.73878518338236	c

-5.62138412970199	3.87459130263793	-4.81991272856135	c
5.38024080104277	3.88328626564364	4.80635891300564	c
-4.68040129548146	5.05461078052645	4.73878518338236	c
5.26508936473195	4.78515797763975	-4.82763136180781	c
5.62138412970199	-3.87459130263793	4.81991272856135	c
6.71551423806347	-3.39463036162852	-6.00783806927879	c
-7.84808611010761	3.76077990453040	-6.68173184049486	c
7.64034881159557	3.50015431981795	6.59374628048872	c
-6.71551423806347	3.39463036162852	6.00783806927879	c
7.70861597603231	3.69422721478108	-5.99957184092069	c
7.84808611010761	-3.76077990453040	6.68173184049486	c
8.40562681216758	-4.54977747862206	-6.49874154391457	h
-8.28818372715470	5.64512066916667	-7.50806969412633	h
8.34043623379443	5.32026320313377	7.38351367489691	h
-8.40562681216758	4.54977747862206	6.49874154391457	h
9.09555830504841	5.22893974889002	-6.38840461550196	h
8.28818372715470	-5.64512066916667	7.50806969412633	h
5.98365397152681	-2.52732316187355	-7.77926366055783	h
-7.37362774258880	2.48431581946634	-8.28210941259451	h
7.07312180844321	2.29582985255632	8.22069066583886	h
-5.98365397152681	2.52732316187355	7.77926366055783	h
7.29633083787534	2.70580724328464	-7.81007404480842	h
7.37362774258880	-2.48431581946634	8.28210941259451	h
7.34172066604382	-1.85244016173382	-4.72897363371576	h
-9.58164807282233	3.00438070929193	-5.76632588098134	h
9.23752898706653	2.54651856655314	5.61668599254945	h
-7.34172066604382	1.85244016173382	4.72897363371576	h
8.61902595581788	2.32862664452599	-4.68806138489106	h
9.58164807282233	-3.00438070929193	5.76632588098134	h
3.75246617682033	-7.15512518724146	-6.52052490193365	c
-3.19925828048065	4.91683720870459	-6.07184310840603	c
3.10755772927470	5.14710474970132	6.12901521662124	c
-3.75246617682033	7.15512518724146	6.52052490193365	c
3.95960183656471	6.68093911179509	-6.60514734505671	c
3.19925828048065	-4.91683720870459	6.07184310840603	c
3.03758871505360	-3.80467461514547	-4.34178221796740	h
-5.20983816487960	1.89777115584508	-4.25437230786461	h
4.74405471134238	1.97387406670576	4.21514404317184	h
-3.03758871505360	3.80467461514547	4.34178221796740	h
3.94194103028989	3.17990294327289	-4.53465759353254	h
5.20983816487960	-1.89777115584508	4.25437230786461	h
2.80778957185671	-6.31112855841501	-8.19777280128819	h
-2.68647555401528	3.78032861252450	-7.76606576475485	h
2.49856719413891	4.02760264814478	7.80275438600242	h
-2.80778957185671	6.31112855841501	8.19777280128819	h
3.38518729746540	5.73237102664844	-8.39159961844077	h
2.68647555401528	-3.78032861252450	7.76606576475485	h
2.36744352368609	-8.41169000016802	-5.56278431063722	h
-1.56736169163070	4.85921392696670	-4.74188507856749	h
1.46596942572889	5.30157035899294	4.82113573326358	h
-2.36744352368609	8.41169000016802	5.56278431063722	h
2.23429723121065	7.48656445571194	-5.71727848547829	h
1.56736169163070	-4.85921392696670	4.74188507856749	h
5.33270257563920	-8.34729035217757	-7.23174243047933	h
-3.46375610490605	6.91405674022596	-6.67546305673728	h
3.59208492151218	7.08724266476860	6.78074251017886	h
-5.33270257563920	8.34729035217757	7.23174243047933	h
5.22835077588340	8.27654499371326	-7.12378722156705	h
3.46375610490605	-6.91405674022596	6.67546305673728	h

13.75372704199694	-0.02818982070191	5.12426703626334	cl
-13.75372704199694	0.02818982070191	-5.12426703626334	cl

[{ClCp$_2$ZrC≡CC(NDipp)$_2$}$_2$Au$_2$] **2** (singlet ground state)

-14.16429064362443	0.03138380389666	-0.95849977104574	zr
-16.63147232485049	-4.05280713784394	-1.45306090068553	c
-17.17157345196932	-3.09658803990183	1.01138400370603	c
-14.89231319116316	-3.22350110468262	2.47038989966274	c
-12.96388290218692	-4.28341229560778	0.91188239102921	c
-14.02743302430296	-4.75664483214776	-1.52016565013819	c
-17.96814028954627	-4.17765314076703	-3.03662450666191	h
-19.02448979688185	-2.44929959852746	1.68550617933708	h
-14.67337763754749	-2.66210156704836	4.45622118797082	h
-10.99873593670513	-4.65836233645752	1.45644333033545	h
-12.99010280901213	-5.49317838692413	-3.15886286812403	h
-0.01377439365904	-2.64011361194655	0.08913375517171	au
-3.89007774015502	-2.23011899819622	0.25409903688024	n
-5.04935042252387	0.04067822817126	0.16396369357132	c
-7.74612987754114	0.04569235547972	-0.00519288243166	c
-10.06623141622750	0.05291180610512	-0.31871201589183	c
-7.31519951776256	-8.11738130866905	2.11711319812785	c
-5.96549912319012	-5.83265814885510	2.32985629534197	c
-5.39337632167803	-4.47803375947933	0.08709352297247	c
-6.17400246486036	-5.36280545526288	-2.32612429548561	c
-7.52092348634175	-7.65388769488933	-2.44282518768097	c
-8.08446100312020	-9.03151682977597	-0.24809815015975	c
-7.79580981599552	-9.18907303952367	3.83747098467683	h
-8.13478898403840	-8.38565522565235	-4.29468234527054	h
-9.14240919272213	-10.82036836909735	-0.38180907197414	h
-5.27425133456125	-4.75564314826488	4.90908381162369	c
-7.65864661297234	-3.63082966105951	6.16494901700190	c
-9.06508018053957	-5.14111982961590	6.57971460105150	h
-7.17627320579097	-2.67142800758385	7.97400977521083	h
-8.57721402489891	-2.22833404739352	4.89979411342248	h
-3.95220576056303	-6.68373822459503	6.64219551790585	c
-3.92848769090494	-3.17789324058293	4.58037991968220	h
-3.30076078391848	-5.75109833687700	8.41125425705516	h
-2.27290653150499	-7.52508819450258	5.70137664673539	h
-5.23745083695515	-8.25526942837338	7.19792248658505	h
-5.49773493197128	-3.92085424326643	-4.72726798478125	c
-3.23632436319647	-5.19486361383545	-6.05677413615456	c
-7.77695402300462	-3.55356786137346	-6.49549890721164	c
-3.70107602450289	-7.16171718668026	-6.63931532058758	h
-8.48802128231548	-5.37551307178606	-7.26929722753482	h
-2.67079308793390	-4.11990246282282	-7.77501586882566	h
-7.24408175105099	-2.35361189288924	-8.13691125691400	h
-1.57286305442921	-5.27850552614086	-4.76929223094418	h
-9.35960846569048	-2.60032148622632	-5.49497115922998	h
-4.85787214997866	-2.00700048504937	-4.15787317115851	h
14.16429064362443	-0.03138380389666	0.95849977104574	zr
16.62912127859122	-4.14651980266364	1.29455157026523	c
-17.24074325789143	3.02431875606920	1.08254926345596	c
17.17157345196932	3.09658803990183	-1.01138400370603	c
-16.62912127859122	4.14651980266364	-1.29455157026523	c
16.63147232485049	4.05280713784394	1.45306090068553	c
17.24074325789143	-3.02431875606920	-1.08254926345596	c

15.00925643395786	-3.06835004656081	-2.62004831919077	c
-14.03037094015807	4.86315278116257	-1.23273274503588	c
14.02743302430296	4.75664483214776	1.52016565013819	c
-15.00925643395786	3.06835004656081	2.62004831919077	c
14.89231319116316	3.22350110468262	-2.47038989966274	c
14.03037094015807	-4.86315278116257	1.23273274503588	c
13.03866344138564	-4.23359276910448	-1.19646019386019	c
-13.03866344138564	4.23359276910448	1.19646019386019	c
12.96388290218692	4.28341229560778	-0.91188239102921	c
17.90846983063291	-4.36395343258197	2.91397393092470	h
-19.10804830555609	2.32635265571024	1.65879772021197	h
19.02448979688185	2.44929959852746	-1.68550617933708	h
-17.90846983063291	4.36395343258197	-2.91397393092470	h
17.96814028954627	4.17765314076703	3.03662450666191	h
19.10804830555609	-2.32635265571024	-1.65879772021197	h
14.85933239885614	-2.38271277669441	-4.57308978986249	h
-12.94311573078365	5.70554831740035	-2.78592496372125	h
12.99010280901213	5.49317838692413	3.15886286812403	h
-14.85933239885614	2.38271277669441	4.57308978986249	h
14.67337763754749	2.66210156704836	-4.45622118797082	h
12.94311573078365	-5.70554831740035	2.78592496372125	h
11.09194247966130	-4.57995857211108	-1.82264134975622	h
-11.09194247966130	4.57995857211108	1.82264134975622	h
10.99873593670513	4.65836233645752	-1.45644333033545	h
0.01377439365904	2.64011361194655	-0.08913375517171	au
3.86938151103607	-2.30277948291551	-0.13309685050043	n
-3.86938151103607	2.30277948291551	0.13309685050043	n
3.89007774015502	2.23011899819622	-0.25409903688024	n
5.04935042252387	-0.04067822817126	-0.16396369357132	c
7.74612987754114	-0.04569235547972	0.00519288243166	c
10.06623141622750	-0.05291180610512	0.31871201589183	c
7.25453987116691	-8.18174805472799	-2.07780730183661	c
-7.68267064768422	7.65447543006785	-2.46146763445788	c
7.52092348634175	7.65388769488933	2.44282518768097	c
-7.25453987116691	8.18174805472799	2.07780730183661	c
7.31519951776256	8.11738130866905	-2.11711319812785	c
7.68267064768422	-7.65447543006785	2.46146763445788	c
5.83273817119021	-5.93776020831378	-2.24645883460587	c
-6.28034951427056	5.39508726845130	-2.38823552233739	c
6.17400246486036	5.36280545526288	2.32612429548561	c
-5.83273817119021	5.93776020831378	2.24645883460587	c
5.96549912319012	5.83265814885510	-2.32985629534197	c
6.28034951427056	-5.39508726845130	2.38823552233739	c
5.37002987934479	-4.55490051962801	0.00495772280749	c
-5.37002987934479	4.55490051962801	-0.00495772280749	c
5.39337632167803	4.47803375947933	-0.08709352297247	c
8.17683269981891	-9.03938588612424	0.25376591921463	c
-8.17683269981891	9.03938588612424	-0.25376591921463	c
8.08446100312020	9.03151682977597	0.24809815015975	c
7.65555492930466	-9.27682603667931	-3.80374547237066	h
-8.40216003133654	8.35151749552034	-4.28763064176910	h
8.13478898403840	8.38565522565235	4.29468234527054	h
-7.65555492930466	9.27682603667931	3.80374547237066	h
7.79580981599552	9.18907303952367	-3.83747098467683	h
8.40216003133654	-8.35151749552034	4.28763064176910	h
9.28712803582505	-10.79943697533335	0.35286710800066	h
-9.28712803582505	10.79943697533335	-0.35286710800066	h
9.14240919272213	10.82036836909735	0.38180907197414	h
4.91537988042906	-4.93087496024636	-4.78445435690545	c

-5.67509629617368	3.93555145722450	-4.79969779815635	c
5.49773493197128	3.92085424326643	4.72726798478125	c
-4.91537988042906	4.93087496024636	4.78445435690545	c
5.27425133456125	4.75564314826488	-4.90908381162369	c
5.67509629617368	-3.93555145722450	4.79969779815635	c
7.06738587895170	-3.46960409179097	-6.10294427083817	c
-7.93934660807817	3.72571127531717	-6.60815118726261	c
7.77695402300462	3.55356786137346	6.49549890721164	c
-7.06738587895170	3.46960409179097	6.10294427083817	c
7.65864661297234	3.63082966105951	-6.16494901700190	c
7.93934660807817	-3.72571127531717	6.60815118726261	c
8.65492643246359	-4.76588535921787	-6.58620185507686	h
-8.49883994031924	5.58855551419394	-7.41021454381397	h
8.48802128231548	5.37551307178606	7.26929722753482	h
-8.65492643246359	4.76588535921787	6.58620185507686	h
9.06508018053957	5.14111982961590	-6.57971460105150	h
8.49883994031924	-5.58855551419394	7.41021454381397	h
6.39247811657752	-2.56778407332511	-7.88072643657570	h
-7.45836987773346	2.47608912472286	-8.22774824651098	h
7.24408175105099	2.35361189288924	8.13691125691400	h
-6.39247811657752	2.56778407332511	7.88072643657570	h
7.17627320579097	2.67142800758385	-7.97400977521083	h
7.45836987773346	-2.47608912472286	8.22774824651098	h
7.82676689875653	-1.96508705751270	-4.85069394625269	h
-9.60774682649285	2.89422057875644	-5.63850204033715	h
9.35960846569048	2.60032148622632	5.49497115922998	h
-7.82676689875653	1.96508705751270	4.85069394625269	h
8.57721402489891	2.22833404739352	-4.89979411342248	h
9.60774682649285	-2.89422057875644	5.63850204033715	h
3.79730954944979	-6.98564519596520	-6.51043533851376	c
-3.32371759435305	5.07630866752621	-6.09703095192433	c
3.23632436319647	5.19486361383545	6.05677413615456	c
-3.79730954944979	6.98564519596520	6.51043533851376	c
3.95220576056303	6.68373822459503	-6.64219551790585	c
3.32371759435305	-5.07630866752621	6.09703095192433	c
3.38251311138513	-3.55304337010987	-4.37997724518438	h
-5.16753173253449	1.97916657308746	-4.24342408387699	h
4.85787214997866	2.00700048504937	4.15787317115851	h
-3.38251311138513	3.55304337010987	4.37997724518438	h
3.92848769090494	3.17789324058293	-4.58037991968220	h
5.16753173253449	-1.97916657308746	4.24342408387699	h
2.91886637841254	-6.10986908544283	-8.20791316993282	h
-2.81339432693954	3.98046078851720	-7.81979363949019	h
2.67079308793390	4.11990246282282	7.77501586882566	h
-2.91886637841254	6.10986908544283	8.20791316993282	h
3.30076078391848	5.75109833687700	-8.41125425705516	h
2.81339432693954	-3.98046078851720	7.81979363949019	h
2.31323265166738	-8.08714839831337	-5.51047487432944	h
-1.66505969034692	5.05056187943407	-4.80113229766855	h
1.57286305442921	5.27850552614086	4.76929223094418	h
-2.31323265166738	8.08714839831337	5.51047487432944	h
2.27290653150499	7.52508819450258	-5.70137664673539	h
1.66505969034692	-5.05056187943407	4.80113229766855	h
5.26099216267459	-8.33571952867484	-7.18972187772026	h
-3.66915427019992	7.07210381616773	-6.66498213581840	h
3.70107602450289	7.16171718668026	6.63931532058758	h
-5.26099216267459	8.33571952867484	7.18972187772026	h
5.23745083695515	8.25526942837338	-7.19792248658505	h
3.66915427019992	-7.07210381616773	6.66498213581840	h

14.33554427846709	-0.14377668898358	5.55991413442110	cl
-14.33554427846709	0.14377668898358	-5.55991413442110	cl

[{ClCp$_2$ZrC≡CC(NDipp)$_2$}$_2$Au$_2$] **2** (triplet state)

-14.17084090076306	0.06646879207972	-1.06857266619108	zr
-17.38568398559682	-3.35829923944908	-0.23325713998465	c
-16.44987690882851	-2.56309477294796	2.18229331266201	c
-13.85633209453693	-3.27289541434004	2.34566806817820	c
-13.19493654702612	-4.55461731130029	0.04843600888764	c
-15.37219164981147	-4.61500725286871	-1.52345444594185	c
-19.31814472660316	-3.09365094863893	-0.94798280167437	h
-17.54530387992813	-1.58881373716817	3.65138122820859	h
-12.57308020476404	-2.92539754972773	3.93894668705535	h
-11.32015416469693	-5.31213504266135	-0.41818202891474	h
-15.46369967940852	-5.39713898156432	-3.44150037047746	h
0.04061422334943	-2.59238049276562	-0.01650750419574	au
-3.81350726732950	-2.32665593787769	0.21674879475164	n
-5.09376786551041	-0.08192262756154	0.09301847879348	c
-7.73634775048124	-0.09883717733200	-0.17428229904860	c
-10.06617345804582	-0.01985875968779	-0.54949590428803	c
-6.85648867464664	-8.41702464338214	1.99302771907226	c
-5.56555103751311	-6.10509511094362	2.22593658376206	c
-5.21427946005042	-4.62803554386003	0.00765730405171	c
-6.09873224402865	-5.43735413153500	-2.39850576967793	c
-7.35063249420977	-7.78010630079018	-2.53121815871174	c
-7.73779114060320	-9.25641287128253	-0.36276068871592	c
-7.18936599102408	-9.58359026134687	3.68426820552983	h
-8.03831001108369	-8.46709845999712	-4.37230965020521	h
-8.74277231248201	-11.07514367698243	-0.50886844249850	h
-4.71527921153067	-5.09583513660237	4.78642333635920	c
-6.87116974860112	-3.53624540100169	5.98458239756384	c
-8.52002223983104	-4.77336841839704	6.40997553252943	h
-6.24491633040496	-2.63465852987708	7.77946891940425	h
-7.52623632447098	-2.02777770027629	4.67912768150300	h
-3.74184692600541	-7.15047116564777	6.59684838662750	c
-3.12346681399066	-3.76957122035743	4.43182713954393	h
-2.88208189724059	-6.26443776853753	8.29792688072836	h
-2.27573816617387	-8.34368252472428	5.67905942816997	h
-5.28451316706640	-8.41341073767044	7.26703365363106	h
-5.57107508613734	-3.90782566935018	-4.78150796907018	c
-3.24195975619960	-4.98974510801977	-6.16591671767933	c
-7.89287338826613	-3.68905321502306	-6.51462131057672	c
-3.58425035295897	-6.96764459975927	-6.79416211785245	h
-8.44494121804030	-5.54248642724536	-7.34235667275141	h
-2.77920170329719	-3.83389243826982	-7.86175170165820	h
-7.47956266070797	-2.39552254757604	-8.11718470270457	h
-1.55227780486803	-4.99710963149200	-4.90951380228635	h
-9.54346157455452	-2.90862700076832	-5.47608957369757	h
-5.07040657853801	-1.95796152061689	-4.19698306288962	h
14.17084090076306	-0.06646879207972	1.06857266619108	zr
16.51300200448634	-4.18256727185205	1.83264596415823	c
-17.18667890986433	3.32951250922270	0.63715278775820	c
16.44987690882851	2.56309477294796	-2.18229331266201	c
-16.51300200448634	4.18256727185205	-1.83264596415823	c
17.38568398559682	3.35829923944908	0.23325713998465	c
17.18667890986433	-3.32951250922270	-0.63715278775820	c
14.97723325199667	-3.46783672070560	-2.20003784167829	c

-13.88917583770903	4.82607420473334	-1.80046217486030	c
15.37219164981147	4.61500725286871	1.52345444594185	c
-14.97723325199667	3.46783672070560	2.20003784167829	c
13.85633209453693	3.27289541434004	-2.34566806817820	c
13.88917583770903	-4.82607420473334	1.80046217486030	c
12.95314015200577	-4.41768382205374	-0.69677886835311	c
-12.95314015200577	4.41768382205374	0.69677886835311	c
13.19493654702612	4.55461731130029	-0.04843600888764	c
17.76588296476861	-4.27159083768508	3.48428282710976	h
-19.07567885692840	2.71245614701622	1.24005535242645	h
17.54530387992813	1.58881373716817	-3.65138122820859	h
-17.76588296476861	4.27159083768508	-3.48428282710976	h
19.31814472660316	3.09365094863893	0.94798280167437	h
19.07567885692840	-2.71245614701622	-1.24005535242645	h
14.86159278402990	-2.95573611122479	-4.20888646295159	h
-12.76168459877606	5.47871158568343	-3.41447560501504	h
15.46369967940852	5.39713898156432	3.44150037047746	h
-14.86159278402990	2.95573611122479	4.20888646295159	h
12.57308020476404	2.92539754972773	-3.93894668705535	h
12.76168459877606	-5.47871158568343	3.41447560501504	h
11.00607861488163	-4.75424370601762	-1.32250848864408	h
-11.00607861488163	4.75424370601762	1.32250848864408	h
11.32015416469693	5.31213504266135	0.41818202891474	h
-0.04061422334943	2.59238049276562	0.01650750419574	au
3.87897011795631	-2.19786635249602	-0.23318297181184	n
-3.87897011795631	2.19786635249602	0.23318297181184	n
3.81350726732950	2.32665593787769	-0.21674879475164	n
5.09376786551041	0.08192262756154	-0.09301847879348	c
7.73634775048124	0.09883717733200	0.17428229904860	c
10.06617345804582	0.01985875968779	0.54949590428803	c
7.20628550887696	-8.14164866299006	-2.02639147282683	c
-7.42694510661611	7.63449831472590	-2.53219009781775	c
7.35063249420977	7.78010630079018	2.53121815871174	c
-7.20628550887696	8.14164866299006	2.02639147282683	c
6.85648867464664	8.41702464338214	-1.99302771907226	c
7.42694510661611	-7.63449831472590	2.53219009781775	c
5.89313123871911	-5.84061683079915	-2.26455676196272	c
-6.12819175736565	5.31841589314798	-2.39553250670425	c
6.09873224402865	5.43735413153500	2.39850576967793	c
-5.89313123871911	5.84061683079915	2.26455676196272	c
5.56555103751311	6.10509511094362	-2.22593658376206	c
6.12819175736565	-5.31841589314798	2.39553250670425	c
5.35273062793511	-4.45891270320585	-0.02862937285799	c
-5.35273062793511	4.45891270320585	0.02862937285799	c
5.21427946005042	4.62803554386003	-0.00765730405171	c
7.96056774110882	-9.04271028441814	0.34969271807842	c
-7.96056774110882	9.04271028441814	-0.34969271807842	c
7.73779114060320	9.25641287128253	0.36276068871592	c
7.68120781022775	-9.23249215239729	-3.73554944160438	h
-8.02833478212826	8.35864386737674	-4.39031935847782	h
8.03831001108369	8.46709845999712	4.37230965020521	h
-7.68120781022775	9.23249215239729	3.73554944160438	h
7.18936599102408	9.58359026134687	-3.68426820552983	h
8.02833478212826	-8.35864386737674	4.39031935847782	h
8.99277560511850	-10.84534065995762	0.50000839405954	h
-8.99277560511850	10.84534065995762	-0.50000839405954	h
8.74277231248201	11.07514367698243	0.50886844249850	h
5.26350156312300	-4.74089148328808	-4.84957661195022	c
-5.46460568777072	3.85325120557729	-4.78476318658176	c

5.57107508613734	3.90782566935018	4.78150796907018	c
-5.26350156312300	4.74089148328808	4.84957661195022	c
4.71527921153067	5.09583513660237	-4.78642333635920	c
5.46460568777072	-3.85325120557729	4.78476318658176	c
7.67815436385808	-3.58770897138051	-6.02050769763871	c
-7.76932125019815	3.42910949033444	-6.50607092108419	c
7.89287338826613	3.68905321502306	6.51462131057672	c
-7.67815436385808	3.58770897138051	6.02050769763871	c
6.87116974860112	3.53624540100169	-5.98458239756384	c
7.76932125019815	-3.42910949033444	6.50607092108419	c
9.09261042736295	-5.09097543296862	-6.43130990824900	h
-8.53416341733922	5.23585384463024	-7.26565426087916	h
8.44494121804030	5.54248642724536	7.34235667275141	h
-9.09261042736295	5.09097543296862	6.43130990824900	h
8.52002223983104	4.77336841839704	-6.40997553252943	h
8.53416341733922	-5.23585384463024	7.26565426087916	h
7.23926310937936	-2.58964721248148	-7.81946780867326	h
-7.23386775200433	2.24142292774954	-8.15488251780730	h
7.47956266070797	2.39552254757604	8.11718470270457	h
-7.23926310937936	2.58964721248148	7.81946780867326	h
6.24491633040496	2.63465852987708	-7.77946891940425	h
7.23386775200433	-2.24142292774954	8.15488251780730	h
8.56780761171083	-2.21634229936307	-4.70062692910038	h
-9.31048240386590	2.43971549260024	-5.47728124058429	h
9.54346157455452	2.90862700076832	5.47608957369757	h
-8.56780761171083	2.21634229936307	4.70062692910038	h
7.52623632447098	2.02777770027629	-4.67912768150300	h
9.31048240386590	-2.43971549260024	5.47728124058429	h
3.99799889782381	-6.65455585095456	-6.63651757296586	c
-3.24642290646814	5.14279398036211	-6.17235748808719	c
3.24195975619960	4.98974510801977	6.16591671767933	c
-3.99799889782381	6.65455585095456	6.63651757296586	c
3.74184692600541	7.15047116564777	-6.59684838662750	c
3.24642290646814	-5.14279398036211	6.17235748808719	c
3.90475451302474	-3.16861036477331	-4.54193741692453	h
-4.78606925264327	1.95587798824874	-4.20282788262088	h
5.07040657853801	1.95796152061689	4.19698306288962	h
-3.90475451302474	3.16861036477331	4.54193741692453	h
3.12346681399066	3.76957122035743	-4.43182713954393	h
4.78606925264327	-1.95587798824874	4.20282788262088	h
3.38231903576635	-5.70453212830984	-8.40845660220235	h
-2.67322788863314	4.02941425528723	-7.86294810288557	h
2.77920170329719	3.83389243826982	7.86175170165820	h
-3.38231903576635	5.70453212830984	8.40845660220235	h
2.88208189724059	6.26443776853753	-8.29792688072836	h
2.67322788863314	-4.02941425528723	7.86294810288557	h
2.30399033115520	-7.51872640261804	-5.74338714507835	h
-1.57001854193145	5.31379161903793	-4.91095155930395	h
1.55227780486803	4.99710963149200	4.90951380228635	h
-2.30399033115520	7.51872640261804	5.74338714507835	h
2.27573816617387	8.34368252472428	-5.67905942816997	h
1.57001854193145	-5.31379161903793	4.91095155930395	h
5.30691151668305	-8.20815887368119	-7.18214999991136	h
-3.76972133597237	7.07716729855941	-6.81107167672502	h
3.58425035295897	6.96764459975927	6.79416211785245	h
-5.30691151668305	8.20815887368119	7.18214999991136	h
5.28451316706640	8.41341073767044	-7.26703365363106	h
3.76972133597237	-7.07716729855941	6.81107167672502	h
14.23177511667007	0.23673843435097	5.72101029158402	cl

-14.23177511667007	-0.23673843435097	-5.72101029158402	cl

[{(PPh_3)AuC≡CC(NDipp)$_2$}$_2$$Au_2$] (singlet ground state)

-13.23368254572728	-1.07084765353185	1.75875098278005	au
0.41568910806506	-2.54738710956562	-0.49351343981216	au
-3.24282118581515	-2.97777594648394	0.78717446786073	n
-4.72059003585185	-1.04694759587074	1.55674321536046	c
-7.29091019933272	-1.59648571978660	2.20573842806274	c
-9.61272560570888	-1.74207491017737	2.46955144257076	c
-5.07906688220048	-9.64670323121924	2.16211913406233	c
-4.05163998761724	-7.21555033279725	2.49976419763024	c
-4.35680295880215	-5.42828024046083	0.52867737393951	c
-5.65263370056951	-6.03797055557146	-1.74150938687390	c
-6.64677878293999	-8.49094822049125	-1.99620740940525	c
-6.36892346654834	-10.28722516926472	-0.06391385439515	c
-4.87637701936926	-11.06382369879053	3.67793332895657	h
-7.66175867285441	-9.00969502339693	-3.74213771571586	h
-7.16674383472929	-12.19901671636401	-0.29432393878746	h
-2.67858620033804	-6.49393928178684	4.92630377450403	c
-4.49648025621263	-6.50445502041266	7.20277859295251	c
-5.21017136512212	-8.44421975967544	7.60472046611454	h
-3.52812536574928	-5.80228160395114	8.93409354071686	h
-6.15721898321074	-5.27210996118459	6.83208744550544	h
-0.33667129478241	-8.16369068285057	5.37296050812917	c
-1.99747000517035	-4.52327222047845	4.68337580951957	h
0.74021529445769	-7.50194678202324	7.05535534092221	h
0.94984380931981	-8.09620241809326	3.71288587732671	h
-0.86550897591781	-10.17475229873449	5.70139189942456	h
-5.91546284596198	-4.10282530084279	-3.86297538176492	c
-4.30288437070667	-4.86869592418109	-6.16462192795732	c
-8.70046659089138	-3.60586755021869	-4.55495899945047	c
-4.94357884510675	-6.69846432920890	-6.98259376456057	h
-9.62770243800524	-5.31037896284469	-5.36995680465260	h
-4.40606378509564	-3.40686138657677	-7.67597266286167	h
-8.84264059669050	-2.06039173102217	-5.97792717811689	h
-2.28554836215650	-5.07961190333227	-5.60713959343463	h
-9.78098005648346	-3.03051690480151	-2.84588014877768	h
-5.12662212682812	-2.29084764142759	-3.16392984552861	h
13.23368254572728	1.07084765353185	-1.75875098278005	au
-0.41568910806506	2.54738710956562	0.49351343981216	au
3.98725034137333	-1.39940774081510	-1.63648600386573	n
-3.98725034137333	1.39940774081510	1.63648600386573	n
3.24282118581515	2.97777594648394	-0.78717446786073	n
4.72059003585185	1.04694759587074	-1.55674321536046	c
7.29091019933272	1.59648571978660	-2.20573842806274	c
9.61272560570888	1.74207491017737	-2.46955144257076	c
7.24279163446347	-6.19524414048902	-5.65257252414542	c
-9.22217228221076	6.14371968969154	1.51053625993327	c
6.64677878293999	8.49094822049125	1.99620740940525	c
-7.24279163446347	6.19524414048902	5.65257252414542	c
5.07906688220048	9.64670323121924	-2.16211913406233	c
9.22217228221076	-6.14371968969154	-1.51053625993327	c
5.54339042153989	-4.28548005801845	-4.91118586370635	c
-7.57025764176538	4.23396156302979	0.67911927619278	c
5.65263370056951	6.03797055557146	1.74150938687390	c
-5.54339042153989	4.28548005801845	4.91118586370635	c
4.05163998761724	7.21555033279725	-2.49976419763024	c

7.57025764176538	-4.23396156302979	-0.67911927619278	c
5.74280516012674	-3.30249572758033	-2.41931865374007	c
-5.74280516012674	3.30249572758033	2.41931865374007	c
4.35680295880215	5.42828024046083	-0.52867737393951	c
9.07513375706733	-7.11354092688999	-3.97371061339518	c
-9.07513375706733	7.11354092688999	3.97371061339518	c
6.36892346654834	10.28722516926472	0.06391385439515	c
7.13630639223851	-6.98225293738226	-7.57693584848096	h
-10.66141439192516	6.89167649790884	0.20860486397545	h
7.66175867285441	9.00969502339693	3.74213771571586	h
-7.13630639223851	6.98225293738226	7.57693584848096	h
4.87637701936926	11.06382369879053	-3.67793332895657	h
10.66141439192516	-6.89167649790884	-0.20860486397545	h
10.39118687315090	-8.61187680918126	-4.58477593689626	h
-10.39118687315090	8.61187680918126	4.58477593689626	h
7.16674383472929	12.19901671636401	0.29432393878746	h
3.56535930874732	-3.22594700396055	-6.72304478476350	c
-7.69469241132856	3.23389252553727	-2.02684772710077	c
5.91546284596198	4.10282530084279	3.86297538176492	c
-3.56535930874732	3.22594700396055	6.72304478476350	c
2.67858620033804	6.49393928178684	-4.92630377450403	c
7.69469241132856	-3.23389252553727	2.02684772710077	c
4.55516234105989	-0.82947800975653	-8.06101170928696	c
-10.34576480592066	3.40048308785500	-3.20500591153784	c
8.70046659089138	3.60586755021869	4.55495899945047	c
-4.55516234105989	0.82947800975653	8.06101170928696	c
4.49648025621263	6.50445502041266	-7.20277859295251	c
10.34576480592066	-3.40048308785500	3.20500591153784	c
6.21904975228311	-1.28907498823619	-9.26402636994972	h
-10.92847246460226	5.38226601992162	-3.60298647440338	h
9.62770243800524	5.31037896284469	5.36995680465260	h
-6.21904975228311	1.28907498823619	9.26402636994972	h
5.21017136512212	8.44421975967544	-7.60472046611454	h
10.92847246460226	-5.38226601992162	3.60298647440338	h
3.06525594217167	0.00757138881469	-9.28918572594535	h
-10.39050113279385	2.36172405536497	-5.03172448140463	h
8.84264059669050	2.06039173102217	5.97792717811689	h
-3.06525594217167	-0.00757138881469	9.28918572594535	h
3.52812536574928	5.80228160395114	-8.93409354071686	h
10.39050113279385	-2.36172405536497	5.03172448140463	h
5.15861827019313	0.63219429029524	-6.68417138746481	h
-11.78990482573395	2.55367132445207	-1.93351148552261	h
9.78098005648346	3.03051690480151	2.84588014877768	h
-5.15861827019313	-0.63219429029524	6.68417138746481	h
6.15721898321074	5.27210996118459	-6.83208744550544	h
11.78990482573395	-2.55367132445207	1.93351148552261	h
2.58004401910406	-5.16628381343105	-8.64892922204981	c
-5.72548217356924	4.56908273035117	-3.71423635268912	c
4.30288437070667	4.86869592418109	6.16462192795732	c
-2.58004401910406	5.16628381343105	8.64892922204981	c
0.33667129478241	8.16369068285057	-5.37296050812917	c
5.72548217356924	-4.56908273035117	3.71423635268912	c
1.92220562875873	-2.63791239851856	-5.54550538346855	h
-7.18958528022685	1.19992706170488	-1.96650548427419	h
5.12662212682812	2.29084764142759	3.16392984552861	h
-1.92220562875873	2.63791239851856	5.54550538346855	h
1.99747000517035	4.52327222047845	-4.68337580951957	h
7.18958528022685	-1.19992706170488	1.96650548427419	h
0.93332577641313	-4.37508143723853	-9.68926608408955	h

-5.75600226466760	3.78213060275327	-5.66526375404526	h
4.40606378509564	3.40686138657677	7.67597266286167	h
-0.93332577641313	4.37508143723853	9.68926608408955	h
-0.74021529445769	7.50194678202324	-7.05535534092221	h
5.75600226466760	-3.78213060275327	5.66526375404526	h
1.95407045777380	-6.93634851881195	-7.70424708143317	h
-3.77968648346123	4.32289385615680	-2.95450981156961	h
2.28554836215650	5.07961190333227	5.60713959343463	h
-1.95407045777380	6.93634851881195	7.70424708143317	h
-0.94984380931981	8.09620241809326	-3.71288587732671	h
3.77968648346123	-4.32289385615680	2.95450981156961	h
4.03563604492023	-5.66861140973794	-10.08303636333665	h
-6.11613961960526	6.63261477929052	-3.82772185420442	h
4.94357884510675	6.69846432920890	6.98259376456057	h
-4.03563604492023	5.66861140973794	10.08303636333665	h
0.86550897591781	10.17475229873449	-5.70139189942456	h
6.11613961960526	-6.63261477929052	3.82772185420442	h
-17.13380041265551	0.22076332236645	0.16420382734793	p
-17.77416630496100	-1.21342732631886	-2.93802534079487	c
-20.22737011723112	-1.91247543761735	-3.70924962386582	c
-20.60845822547483	-2.95750396311138	-6.12171926172362	c
-18.55246347987719	-3.30927227087489	-7.76606911459404	c
-16.10331867019974	-2.61896985009650	-6.99642633629694	c
-15.70859749672034	-1.57949317130100	-4.59030865543741	c
-21.84405696248373	-1.65513553157384	-2.42038241095067	h
-22.52791159877668	-3.50958138491252	-6.71428648097949	h
-18.85681960903071	-4.13981965757750	-9.65247024304969	h
-14.47675646760090	-2.90960475113284	-8.26471923701880	h
-13.78083574221626	-1.06536894690839	-3.99178694602963	h
-17.15576140643054	3.64580634450279	-0.42150206818484	c
-19.94653739012859	-0.42520856820915	2.08630811681887	c
-18.41824858482032	4.70606493840767	-2.51728029024896	c
-22.06636534721763	1.19184380550775	2.09212362308720	c
-18.40182581296557	7.33572439016740	-2.88129284568824	c
-24.19908124775707	0.57005560334107	3.54617319626916	c
-17.13025884169752	8.91286656672508	-1.16184046780034	c
-24.22461592081149	-1.65758100751616	4.99417446504890	c
-15.86128940265423	7.85695519757703	0.91994736527622	c
-22.10841726342678	-3.26561032938416	4.99933030335776	c
-15.85851471009006	5.23067421816244	1.28816058964008	c
-19.96841562347074	-2.65020629478031	3.55752957227452	c
-19.39532446873453	3.47212456425133	-3.88256031853102	h
-22.04573365581732	2.94669954750573	0.96932828062064	h
-19.37930272193076	8.15604395853423	-4.52800633756780	h
-25.84963903385016	1.84125373812629	3.55485491722385	h
-17.11078551337467	10.97497503735243	-1.45775153361762	h
-25.89826345498794	-2.13632106212644	6.13888260177743	h
-14.83169661040044	9.07943173378357	2.25512785130311	h
-22.11469023274934	-5.00229596406059	6.14918850920814	h
-14.79382999299201	4.41044645150935	2.88198248191221	h
-18.29223175446177	-3.89090525316439	3.58029991018210	h
17.13380041265551	-0.22076332236645	-0.16420382734793	p
17.77416630496100	1.21342732631886	2.93802534079487	c
20.22737011723112	1.91247543761735	3.70924962386582	c
20.60845822547483	2.95750396311138	6.12171926172362	c
18.55246347987719	3.30927227087489	7.76606911459404	c
16.10331867019974	2.61896985009650	6.99642633629694	c
15.70859749672034	1.57949317130100	4.59030865543741	c
21.84405696248373	1.65513553157384	2.42038241095067	h

22.52791159877668	3.50958138491252	6.71428648097949	h
18.85681960903071	4.13981965757750	9.65247024304969	h
14.47675646760090	2.90960475113284	8.26471923701880	h
13.78083574221626	1.06536894690839	3.99178694602963	h
17.15576140643054	-3.64580634450279	0.42150206818484	c
19.94653739012859	0.42520856820915	-2.08630811681887	c
18.41824858482032	-4.70606493840767	2.51728029024896	c
22.06636534721763	-1.19184380550775	-2.09212362308720	c
18.40182581296557	-7.33572439016740	2.88129284568824	c
24.19908124775707	-0.57005560334107	-3.54617319626916	c
17.13025884169752	-8.91286656672508	1.16184046780034	c
24.22461592081149	1.65758100751616	-4.99417446504890	c
15.86128940265423	-7.85695519757703	-0.91994736527622	c
22.10841726342678	3.26561032938416	-4.99933030335776	c
15.85851471009006	-5.23067421816244	-1.28816058964008	c
19.96841562347074	2.65020629478031	-3.55752957227452	c
19.39532446873453	-3.47212456425133	3.88256031853102	h
22.04573365581732	-2.94669954750573	-0.96932828062064	h
19.37930272193076	-8.15604395853423	4.52800633756780	h
25.84963903385016	-1.84125373812629	-3.55485491722385	h
17.11078551337467	-10.97497503735243	1.45775153361762	h
25.89826345498794	2.13632106212644	-6.13888260177743	h
14.83169661040044	-9.07943173378357	-2.25512785130311	h
22.11469023274934	5.00229596406059	-6.14918850920814	h
14.79382999299201	-4.41044645150935	-2.88198248191221	h
18.29223175446177	3.89090525316439	-3.58029991018210	h

[{(PPh_3)AuC≡CC(NDipp)$_2$}$_2$$Au_2$] (triplet state)

-13.27177703951608	-0.97275192762990	1.65644424558337	au
0.32427000415103	-2.46822676636422	-0.72694802950428	au
-3.29884983438752	-2.91414206143430	0.52155373260655	n
-4.81026749908544	-1.01920223831037	1.41787292347635	c
-7.32639625125604	-1.56456311624054	2.10180989813416	c
-9.66426861632578	-1.65965350028975	2.40094755965574	c
-4.98421310718088	-9.58814575947143	2.00691493762241	c
-3.98055461521256	-7.14115797302230	2.29431972740678	c
-4.38463941173099	-5.38436216755857	0.31359932958003	c
-5.75004510991225	-6.01684949489714	-1.90507770084280	c
-6.70677683805186	-8.48867118061548	-2.10907325529607	c
-6.33437759042500	-10.26320096992787	-0.17251637382966	c
-4.71598674956205	-10.98849002210039	3.52692172893039	h
-7.76632690002275	-9.03920646147935	-3.81725262067439	h
-7.10786375392827	-12.18861990443899	-0.36312770192534	h
-2.56746266398478	-6.36902746754874	4.68334909871414	c
-4.36116922118384	-6.31895033540308	6.97961564774242	c
-5.07784128488940	-8.24612131212250	7.43098162306243	h
-3.36861762209910	-5.58375339751622	8.68280290347576	h
-6.01984495191903	-5.08731655278362	6.59803461020766	h
-0.22407819160294	-8.03326070074677	5.13916711281654	c
-1.88156719564848	-4.40479606964631	4.39721070252299	h
0.87079824057874	-7.33566808816060	6.79441195815605	h
1.04569781811920	-8.00681874396780	3.46435942836924	h
-0.75096012580622	-10.03486914290132	5.51951851854832	h
-6.10060747672657	-4.09801928564602	-4.02739931462095	c
-4.54724817618893	-4.85660202515476	-6.37302068803291	c
-8.91045830180378	-3.64684015945762	-4.63811790750247	c
-5.19943769626699	-6.69269689759667	-7.16577926945445	h

-9.83796012670341	-5.37158564182257	-5.40675996009277	h
-4.71195423941815	-3.40058603408467	-7.88368151497889	h
-9.11525286151094	-2.12191462210229	-6.07391215457569	h
-2.51114439232989	-5.05521033315777	-5.88175137565523	h
-9.94950226504475	-3.06592411943474	-2.90563539776683	h
-5.31793628509248	-2.26929254477350	-3.36131401059185	h
13.27177703951608	0.97275192762990	-1.65644424558337	au
-0.32427000415103	2.46822676636422	0.72694802950428	au
3.94985800443737	-1.42431404721388	-1.64189954934849	n
-3.94985800443737	1.42431404721388	1.64189954934849	n
3.29884983438752	2.91414206143430	-0.52155373260655	n
4.81026749908544	1.01920223831037	-1.41787292347635	c
7.32639625125604	1.56456311624054	-2.10180989813416	c
9.66426861632578	1.65965350028975	-2.40094755965574	c
7.09251554115667	-6.51357177880021	-5.33621562073118	c
-9.15114021623259	6.18069793389025	1.23949863739829	c
6.70677683805186	8.48867118061548	2.10907325529607	c
-7.09251554115667	6.51357177880021	5.33621562073118	c
4.98421310718088	9.58814575947143	-2.00691493762241	c
9.15114021623259	-6.18069793389025	-1.23949863739829	c
5.41750075735652	-4.54677973550983	-4.71038672380660	c
-7.53976125986278	4.19914729050948	0.51211327807212	c
5.75004510991225	6.01684949489714	1.90507770084280	c
-5.41750075735652	4.54677973550983	4.71038672380660	c
3.98055461521256	7.14115797302230	-2.29431972740678	c
7.53976125986278	-4.19914729050948	-0.51211327807212	c
5.67846312139258	-3.38410495037643	-2.29133047722201	c
-5.67846312139258	3.38410495037643	2.29133047722201	c
4.38463941173099	5.38436216755857	-0.31359932958003	c
8.94649890463629	-7.32249953624851	-3.62383427657903	c
-8.94649890463629	7.32249953624851	3.62383427657903	c
6.33437759042500	10.26320096992787	0.17251637382966	c
6.96113444705751	-7.42647043410702	-7.20091672681714	h
-10.60953904113839	6.85358705703010	-0.07985030624224	h
7.76632690002275	9.03920646147935	3.81725262067439	h
-6.96113444705751	7.42647043410702	7.20091672681714	h
4.71598674956205	10.98849002210039	-3.52692172893039	h
10.60953904113839	-6.85358705703010	0.07985030624224	h
10.24244938240681	-8.86835639435738	-4.14858909480888	h
-10.24244938240681	8.86835639435738	4.14858909480888	h
7.10786375392827	12.18861990443899	0.36312770192534	h
3.46861757031263	-3.56095715110392	-6.59520026117233	c
-7.69504714045076	3.04904142399539	-2.13176262182551	c
6.10060747672657	4.09801928564602	4.02739931462095	c
-3.46861757031263	3.56095715110392	6.59520026117233	c
2.56746266398478	6.36902746754874	-4.68334909871414	c
7.69504714045076	-3.04904142399539	2.13176262182551	c
4.42656944002831	-1.12967453821461	-7.89520796708333	c
-10.27737354587580	3.41253249605030	-3.41280232294285	c
8.91045830180378	3.64684015945762	4.63811790750247	c
-4.42656944002831	1.12967453821461	7.89520796708333	c
4.36116922118384	6.31895033540308	-6.97961564774242	c
10.27737354587580	-3.41253249605030	3.41280232294285	c
6.15201157238965	-1.53155545452895	-9.02854482397335	h
-10.63055653106531	5.41515804371714	-3.94955830803529	h
9.83796012670341	5.37158564182257	5.40675996009277	h
-6.15201157238965	1.53155545452895	9.02854482397335	h
5.07784128488940	8.24612131212250	-7.43098162306243	h
10.63055653106531	-5.41515804371714	3.94955830803529	h

2.95686126380209	-0.35135179969750	-9.18412294678815	h
-10.36159934585425	2.27456388601519	-5.17687044657423	h
9.11525286151094	2.12191462210229	6.07391215457569	h
-2.95686126380209	0.35135179969750	9.18412294678815	h
3.36861762209910	5.58375339751622	-8.68280290347576	h
10.36159934585425	-2.27456388601519	5.17687044657423	h
4.92486275982187	0.35445134898938	-6.49896441813887	h
-11.84658314456560	2.78846390582436	-2.16193536408195	h
9.94950226504475	3.06592411943474	2.90563539776683	h
-4.92486275982187	-0.35445134898938	6.49896441813887	h
6.01984495191903	5.08731655278362	-6.59803461020766	h
11.84658314456560	-2.78846390582436	2.16193536408195	h
2.61153705986008	-5.52746741226862	-8.55371380591528	c
-5.55594448520382	4.05072999226864	-3.84585434210524	c
4.54724817618893	4.85660202515476	6.37302068803291	c
-2.61153705986008	5.52746741226862	8.55371380591528	c
0.22407819160294	8.03326070074677	-5.13916711281654	c
5.55594448520382	-4.05072999226864	3.84585434210524	c
1.75721128432528	-3.02644292372854	-5.48596226254403	h
-7.42426360230695	0.97983002080621	-1.92522620040608	h
5.31793628509248	2.26929254477350	3.36131401059185	h
-1.75721128432528	3.02644292372854	5.48596226254403	h
1.88156719564848	4.40479606964631	-4.39721070252299	h
7.42426360230695	-0.97983002080621	1.92522620040608	h
0.98772205815707	-4.77624121715278	-9.65675921277062	h
-5.62766846069745	3.11808871757764	-5.72960846781730	h
4.71195423941815	3.40058603408467	7.88368151497889	h
-0.98772205815707	4.77624121715278	9.65675921277062	h
-0.87079824057874	7.33566808816060	-6.79441195815605	h
5.62766846069745	-3.11808871757764	5.72960846781730	h
1.99409837844003	-7.31371051793250	-7.63460616399947	h
-3.65643453097804	3.68080557865952	-3.02491031612080	h
2.51114439232989	5.05521033315777	5.88175137565523	h
-1.99409837844003	7.31371051793250	7.63460616399947	h
-1.04569781811920	8.00681874396780	-3.46435942836924	h
3.65643453097804	-3.68080557865952	3.02491031612080	h
4.13391057140114	-5.98625924603158	-9.93057519148083	h
-5.73735171592028	6.12545473064223	-4.13057772268100	h
5.19943769626699	6.69269689759667	7.16577926945445	h
-4.13391057140114	5.98625924603158	9.93057519148083	h
0.75096012580622	10.03486914290132	-5.51951851854832	h
5.73735171592028	-6.12545473064223	4.13057772268100	h
-17.22642893606009	0.27392503386470	0.14419865705716	p
-17.85572306789629	-1.15702620014904	-2.97330509096266	c
-20.32224453113512	-1.79694330223733	-3.76140511456381	c
-20.72473934648429	-2.78672422805081	-6.19233340375159	c
-18.67668643314389	-3.14538077177660	-7.84754762099461	c
-16.21530084429900	-2.51207357473662	-7.06472164965835	c
-15.80338933247833	-1.51987266853635	-4.64175647515073	c
-21.93014724773126	-1.53700676912651	-2.46127801963254	h
-22.65516050756272	-3.29050636179620	-6.79381573353179	h
-18.99850588943080	-3.92833069820003	-9.75154137649002	h
-14.59557411314277	-2.80553945418163	-8.34230267897659	h
-13.87118609653414	-1.03553217820315	-4.03170995668742	h
-17.33225873583075	3.69253235126294	-0.36943705810777	c
-20.02905924046492	-0.52744004677568	2.02759646285139	c
-18.95848976148575	4.76549707178173	-2.20585532619064	c
-21.88739382602880	1.26771593497256	2.69493127885912	c
-19.02641772046326	7.39572486052568	-2.54579476705894	c

-23.95148454655316	0.54339567365677	4.19905811932768	c
-17.48482652749845	8.98172718164154	-1.07148748393097	c
-24.17964973462283	-1.96588640962473	5.04932894770034	c
-15.85793211973677	7.91872029493133	0.75139655764114	c
-22.32070292861253	-3.75652038736935	4.39801303199333	c
-15.77293152182916	5.29334023098749	1.09736616973047	c
-20.24879040241211	-3.04383635996334	2.90931119601627	c
-20.15633514625705	3.53400492855182	-3.38461073943145	h
-21.71584731066655	3.23734019676493	2.03913866320324	h
-20.29050105603035	8.21471391636732	-3.98610165746793	h
-25.39660167854369	1.95489174579835	4.71017092319114	h
-17.54028152841794	11.04564299539766	-1.34757404549052	h
-25.79863806170432	-2.52587488483122	6.23455298928040	h
-14.63603790479540	9.14549853495473	1.91038979751029	h
-22.48188905101376	-5.72229347966375	5.07028996141726	h
-14.46293828941002	4.47651910548857	2.50011041122353	h
-18.77784253498655	-4.44134988539428	2.42504202101554	h
17.22642893606009	-0.27392503386470	-0.14419865705716	p
17.85572306789629	1.15702620014904	2.97330509096266	c
20.32224453113512	1.79694330223733	3.76140511456381	c
20.72473934648429	2.78672422805081	6.19233340375159	c
18.67668643314389	3.14538077177660	7.84754762099461	c
16.21530084429900	2.51207357473662	7.06472164965835	c
15.80338933247833	1.51987266853635	4.64175647515073	c
21.93014724773126	1.53700676912651	2.46127801963254	h
22.65516050756272	3.29050636179620	6.79381573353179	h
18.99850588943080	3.92833069820003	9.75154137649002	h
14.59557411314277	2.80553945418163	8.34230267897659	h
13.87118609653414	1.03553217820315	4.03170995668742	h
17.33225873583075	-3.69253235126294	0.36943705810777	c
20.02905924046492	0.52744004677568	-2.02759646285139	c
18.95848976148575	-4.76549707178173	2.20585532619064	c
21.88739382602880	-1.26771593497256	-2.69493127885912	c
19.02641772046326	-7.39572486052568	2.54579476705894	c
23.95148454655316	-0.54339567365677	-4.19905811932768	c
17.48482652749845	-8.98172718164154	1.07148748393097	c
24.17964973462283	1.96588640962473	-5.04932894770034	c
15.85793211973677	-7.91872029493133	-0.75139655764114	c
22.32070292861253	3.75652038736935	-4.39801303199333	c
15.77293152182916	-5.29334023098749	-1.09736616973047	c
20.24879040241211	3.04383635996334	-2.90931119601627	c
20.15633514625705	-3.53400492855182	3.38461073943145	h
21.71584731066655	-3.23734019676493	-2.03913866320324	h
20.29050105603035	-8.21471391636732	3.98610165746793	h
25.39660167854369	-1.95489174579835	-4.71017092319114	h
17.54028152841794	-11.04564299539766	1.34757404549052	h
25.79863806170432	2.52587488483122	-6.23455298928040	h
14.63603790479540	-9.14549853495473	-1.91038979751029	h
22.48188905101376	5.72229347966375	-5.07028996141726	h
14.46293828941002	-4.47651910548857	-2.50011041122353	h
18.77784253498655	4.44134988539428	-2.42504202101554	h

X. References

1. T. J. Feuerstein, M. Poß, T. P. Seifert, S. Bestgen, C. Feldmann and P. W. Roesky, *Chem. Commun.*, 2017, **53**, 9012-9015.
2. T. J. Feuerstein, T. P. Seifert, A. P. Jung, R. Müller, S. Lebedkin, M. M. Kappes and P. W. Roesky, *Chem. Eur. J.*, 2020, **26**, 16676-16682.
3. G. M. Sheldrick, *Acta Crystallogr A*, 2008, **64**, 112-122.
4. G. M. Sheldrick, *Acta Crystallogr. Sect. C*, 2015, **71**, 3-8.
5. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.
6. J. C. de Mello, H. F. Wittmann and R. H. Friend, *Adv. Mater.*, 1997, **9**, 230-232.
7. R. Ahlrichs, M. Bär, M. Häser, H. Horn and C. Kölmel, *Chem. Phys. Lett.*, 1989, **162**, 165-169.
8. A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.
9. J. P. Perdew, *Phys. Rev. B*, 1986, **34**, 7406-7406.
10. J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822-8824.
11. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
12. F. Weigend, M. Häser, H. Patzelt and R. Ahlrichs, *Chem. Phys. Lett.*, 1998, **294**, 143-152.