Organometallic Wheels Based on Coinage Metal Ions and Norbornene: Syntheses and Structural Characterization of $[M(norbornene)_3][SbF_6]$ (M = Au, Ag, Cu)

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Supporting Material

Experimental:

All manipulations were carried out under an atmosphere of purified nitrogen using standard Schlenk techniques or in a Vacuum Atmosphere single-station dry-box equipped with a -25 °C refrigerator. Solvents were purchased from commercial sources, purified using Innovative Technology SPS-400 PureSolv solvent drying system or by distilling over conventional drying agents and degassed by the freeze-pump-thaw method prior to use. Glassware was oven-dried at 150 °C overnight. NMR spectra were recorded on a JEOL Eclipse 500 or JEOL Eclipse 300 spectrometer (^{1}H, 500.16 MHz or 300.53 MHz; ^{13}C, 125.78 MHz or 75.59 MHz). Proton and carbon chemical shifts are reported in ppm versus Me_4Si, and referenced using the residual proton or carbon signals of the deuterated solvent. Elemental analyses were performed using a Perkin Elmer Series II CHNS/O analyzer. Raman spectra were recorded at room temperature on Horiba Jobin Yvon LabRAM Aramis instrument using two different laser sources, 473 nm and 633 nm. Crystals of the samples were sealed tight under argon or nitrogen (depending on their reactivity) in a quartz cuvette by the mean of a greased Teflon cap. Different experimental settings (laser intensity, level of magnification, time of exposure, number of cycles) were

used for each compound in order to obtain the best signal-to-noise ratio. Norbornene, AuCl, CuBr and $AgSbF_6$ were purchased from commercial sources and used as received.

Norbornene (C_7H_{10}): ^{1}H NMR (CD_2Cl_2, 298 K): δ 0.94 (t, 2H), 1.10 (d, 1H), 1.29 (d, 1H), 1.61 (t, 2H), 2.84 (s, 2H), 5.98 (s, 2H). ^{13}C {^{1}H} NMR (CD_2Cl_2, 298 K): δ 25.2, 42.5, 49.1, 135.9. Raman: 1565 cm^{-1} (C=C stretch).

[Ag(norbornene)$_3$][SbF$_6$]: $AgSbF_6$ 98% (0.400 g, 1.14 mmol) was placed in a flask with magnetic stir bar. Norbornene C_7H_{10} (0.500g, 5.3 mmol) and dichloromethane (30 mL) was mixed at room temperature in another flask. The norbornene solution was transferred to the flask containing the silver salt. The reaction was immediate. The flask was covered with aluminum foil to protect from the light, and the mixture was stirred overnight at room temperature. The resulting mixture was placed in a -20 °C freezer for a couple of days. Crystals of $[Ag(norbornene)_3][SbF_6]$ formed at the bottom of the flask was separated by filtration. The filtrate was concentrated under reduced pressure to ~2 mL and placed in the -20 °C freezer to obtain a second batch of the compound as a white solid. Overall yield, 0.336 g, 46%. X-ray quality crystals were grown using dilute dichloromethane solution of $[Ag(norbornene)_3][SbF_6]$ at -20°C. ^{1}H NMR (CD_2Cl_2, 298 K): δ 0.84 (m, 1H), 1.01 (m, 2H), 1.18 (m, 1H), 1.77 (m, 2H), 3.20 (s, 2H), 6.42 (s, 2H). ^{13}C {^{1}H} NMR (CD_2Cl_2, 298 K): δ 23.6, 43.7, 48.5, 132.6. Raman: 1507 cm^{-1} (C=C stretch). Elemental analysis: calculated, C 40.29%, H, 4.83%, found, C 40.27%, H 4.85%. Solid $[Ag(norbornene)_3][SbF_6]$ slowly turns tan if left exposed to air/light at room temperature. It is best stored under nitrogen, protected from light, in a low temperature freezer.

[Cu(norbornene)$_3$][SbF$_6$]: $[Ag(norbornene)_3][SbF_6]$ (0.200 g, 0.32 mmol) and CuBr (0.069 g, 0.48 mmol) were placed in a flask with a magnetic stir bar. Dichloromethane (50 mL) was added at room temperature. The reaction flask was covered with aluminum foil to protect from the light and stirred for three hours. The resulting greenish precipitate (presumably containing AgBr plus excess of CuBr) was removed by filtering through a Celite bed. The filtrate was placed in a -20 °C freezer. Crystalline

$[Cu(norbornene)_3][SbF_6]$ (0.120 g) was precipitated from this mixture after about 5 days (yield 65%). X-ray quality colorless crystals can be obtained from a CH_2Cl_2/hexafluorobenzene (50%:50%) solution at -20 °C. This compound appears to be the most stable among the Au, Ag, and Cu norbornene adducts described here. However, it is best stored under nitrogen, in a low temperature freezer. ^{1}H NMR (CD_2Cl_2, 298 K): δ 0.53 (d, 1H), 1.12 (s, 3H), 1.77 (d, 2H), 3.23 (s, 2H), 5.77 (s, 2H). ^{13}C {^{1}H} NMR (CD_2Cl_2, 298 K): δ 24.7, 44.2, 45.9, 122.1. Raman: 1491 cm^{-1} (C=C stretching). Elemental analysis: calculated, C 43.36%, H, 5.20%, found, C 44.05%, H 5.59%.

$[Au(norbornene)_3][SbF_6]$: $AgSbF_6$ 98% (0.140 g, 0.4 mmol) and norbornene C_7H_{10} (0.175 g, 1.8 mmol) were placed in a flask with a magnetic stir bar. Dichloromethane (20 mL) was added at room temperature and stirred for a few minutes to obtain a clear solution. AuCl (0.115 g, 0.48 mmol) and norbornene C_7H_{10} (0.068 g, 0.7 mmol) were placed in a separate flask and dichloromethane (20 mL) was added and the mixture was stirred for a few minutes (~10 min) to get a clear solution. The $AgSbF_6$/norbornene solution was then cooled to -30 ^{o}C using a dry ice-acetone bath and treated with the AuCl/norbornene solution. The resulting mixture was protected from light (using aluminum foil) and stirred for 2 hrs at -30 ^{o}C and addition 3 hrs at about 0 ^{o}C. The mixture was filtered through a Celite bed to remove the resulting grey precipitate, and the filtrate was collected and concentrated under reduced pressure to about 5 mL. $[Au(norbornene)_3][SbF_6]$ precipitates as a white solid. The supernatant was removed and the precipitate was dried under reduced pressure to obtain 0.115 g of $[Au(norbornene)_3][SbF_6]$. Yield: 41 %. Mp: >80 ^{o}C (decomp.). Additional product could be obtained from the supernatant if necessary, since it contains mostly $[Au(norbornene)_3][SbF_6]$ based on the NMR data. ^{1}H NMR (CD_2Cl_2, 298 K): δ 0.49 (m, 1H), 0.78 (m, 1H), 1.15 (m, 2H), 1.88 (m, 2H), 3.30 (s, 2H), 5.53 (s, 2H). ^{13}C{^{1}H} NMR (CD_2Cl_2, 298 K): δ 25.2, 43.8, 44.1, 112.6 (br); ^{1}H NMR (CD_2Cl_2, 273 K): δ 0.34 (m, 1H), 0.70 (m, 1H), 1.17 (m, 2H), 1.86 (m, 2H), 3.28 (s, 2H), 5.38 (s, 2H). ^{13}C{^{1}H} NMR (CD_2Cl_2, 273 K): δ 25.2, 43.2, 43.4, 109.2 (br). Solubility of $[Au(norbornene)_3][SbF_6]$ in CD_2Cl_2 drops significantly upon cooling, which presents difficulties when collecting ^{13}C data at low temperatures (even below -20 °C). Elemental analysis: calculated, C 35.27%, H

4.23%, found, 35.37%, H 4.32%. X-ray quality colorless crystals can be obtained from a CH_2Cl_2/hexafluorobenzene (50%:50%) solution at -20°C. Solid [Au(norbornene)$_3$][SbF_6] slowly turns slightly pink (at least the surface) if left exposed to air/light at room temperature. It is best stored under nitrogen, protected from light, in a low temperature freezer.

One of our first attempts at the synthesis of [Au(norbornene)$_3$][SbF_6] show that it can also be synthesized using [Ag(norbornene)$_3$][SbF_6] and AuCl but the reaction is not clean. For example, a mixture of [Ag(norbornene)$_3$][SbF_6] (0.200 g, 0.32 mmol) and AuCl (0.115 g, 0.48 mmol) in dichloromethane (30 mL) at room temperature also gave [Au(norbornene)$_3$][SbF_6] in low yield along with some decomposition products.

X-ray crystallography:

A suitable crystal of the compound of interest, covered with a layer of hydrocarbon oil, was selected and mounted with paratone-N oil in a cryo-loop and immediately placed in the low-temperature nitrogen stream for the low temperature work. The X-ray intensity data were measured at 100(2) K on a Bruker SMART APEX CCD area detector system equipped with a Oxford Cryosystems 700 Series cooler, a graphite monochromator, and a Mo Kα fine-focus sealed tube (λ = 0.71073 Å). The data frames were integrated with the Bruker SAINT-Plus software package. Data were corrected for absorption effects using the multi-scan technique (SADABS). Structures were solved and refined using Bruker SHELXTL (Version 6.14) software package. Crystal data and some experimental details are summarized in Tables S1-6. Additional details are given below and in the cif files (CCDC 741041 - 741043 contain the supplementary crystallographic data. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge, CB2 1EZ, UK).

Table S1. Crystal data and structure refinement for [Cu(norbornene)$_3$][SbF$_6$], dias591s.

Identification code	dias591s	
Empirical formula	C21 H30 Cu F6 Sb	
Formula weight	581.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R3	
Unit cell dimensions	a = 11.3580(3) Å	α= 90°.
	b = 11.3580(3) Å	β= 90°.
	c = 14.0341(7) Å	γ = 120°.
Volume	1567.90(10) Å^3	
Z	3	
Density (calculated)	1.848 Mg/m^3	
Absorption coefficient	2.367 mm^{-1}	
F(000)	870	
Crystal size	0.13 x 0.13 x 0.12 mm^3	
Theta range for data collection	2.53 to 28.29°.	
Index ranges	-15<=h<=15, -14<=k<=15, -18<=l<=18	
Reflections collected	4876	
Independent reflections	1723 [R(int) = 0.0329]	
Completeness to theta = 28.29°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7643 and 0.7484	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1723 / 1 / 95	
Goodness-of-fit on F^2	1.129	
Final R indices [I>2sigma(I)]	R1 = 0.0276, wR2 = 0.0731	
R indices (all data)	R1 = 0.0276, wR2 = 0.0731	
Absolute structure parameter	0.00(3)	
Largest diff. peak and hole	0.830 and -0.953 e.Å^{-3}	

Table S2. Bond lengths [Å] and angles [°] for [Cu(norbornene)$_3$][SbF$_6$], dias591s.

Cu-C(1)#1	2.197(4)	C(2)-C(3)	1.511(6)
Cu-C(1)#2	2.197(4)	C(2)-H(2)	0.96(9)
Cu-C(1)	2.197(4)	C(3)-C(7)	1.545(6)
Cu-C(2)#1	2.199(4)	C(3)-C(4)	1.564(6)
Cu-C(2)#2	2.199(4)	C(3)-H(3)	1.0000
Cu-C(2)	2.199(4)	C(4)-C(5)	1.548(6)
Sb-F(2)#2	1.867(3)	C(4)-H(4A)	0.9900
Sb-F(2)	1.867(3)	C(4)-H(4B)	0.9900
Sb-F(2)#1	1.867(3)	C(5)-C(6)	1.554(6)
Sb-F(1)#2	1.886(3)	C(5)-H(5A)	0.9900
Sb-F(1)	1.886(3)	C(5)-H(5B)	0.9900
Sb-F(1)#1	1.886(3)	C(6)-C(7)	1.532(6)
C(1)-C(2)	1.378(6)	C(6)-H(6)	1.0000
C(1)-C(6)	1.522(6)	C(7)-H(7A)	0.9900
C(1)-H(1)	0.97(8)	C(7)-H(7B)	0.9900
C(1)#1-Cu-C(1)#2	119.953(9)	C(1)#2-Cu-C(2)#1	155.22(16)
C(1)#1-Cu-C(1)	119.953(9)	C(1)-Cu-C(2)#1	84.45(16)
C(1)#2-Cu-C(1)	119.953(9)	C(1)#1-Cu-C(2)#2	84.45(16)
C(1)#1-Cu-C(2)#1	36.53(16)	C(1)#2-Cu-C(2)#2	36.53(16)

C(1)-Cu-C(2)#2	155.22(16)	C(3)-C(2)-H(2)	111(6)
C(2)#1-Cu-C(2)#2	118.69(5)	Cu-C(2)-H(2)	98(6)
C(1)#1-Cu-C(2)	155.22(16)	C(2)-C(3)-C(7)	100.4(3)
C(1)#2-Cu-C(2)	84.45(16)	C(2)-C(3)-C(4)	104.4(4)
C(1)-Cu-C(2)	36.53(16)	C(7)-C(3)-C(4)	99.4(3)
C(2)#1-Cu-C(2)	118.69(5)	C(2)-C(3)-H(3)	116.7
C(2)#2-Cu-C(2)	118.69(5)	C(7)-C(3)-H(3)	116.7
F(2)#2-Sb-F(2)	90.75(16)	C(4)-C(3)-H(3)	116.7
F(2)#2-Sb-F(2)#1	90.75(16)	C(5)-C(4)-C(3)	103.4(3)
F(2)-Sb-F(2)#1	90.75(16)	C(5)-C(4)-H(4A)	111.1
F(2)#2-Sb-F(1)#2	90.19(18)	C(3)-C(4)-H(4A)	111.1
F(2)-Sb-F(1)#2	90.55(18)	C(5)-C(4)-H(4B)	111.1
F(2)#1-Sb-F(1)#2	178.39(19)	C(3)-C(4)-H(4B)	111.1
F(2)#2-Sb-F(1)	178.39(19)	H(4A)-C(4)-H(4B)	109.0
F(2)-Sb-F(1)	90.19(18)	C(4)-C(5)-C(6)	103.3(3)
F(2)#1-Sb-F(1)	90.55(18)	C(4)-C(5)-H(5A)	111.1
F(1)#2-Sb-F(1)	88.49(16)	C(6)-C(5)-H(5A)	111.1
F(2)#2-Sb-F(1)#1	90.55(18)	C(4)-C(5)-H(5B)	111.1
F(2)-Sb-F(1)#1	178.4(2)	C(6)-C(5)-H(5B)	111.1
F(2)#1-Sb-F(1)#1	90.19(18)	H(5A)-C(5)-H(5B)	109.1
F(1)#2-Sb-F(1)#1	88.49(16)	C(1)-C(6)-C(7)	101.6(3)
F(1)-Sb-F(1)#1	88.49(16)	C(1)-C(6)-C(5)	103.4(3)
C(2)-C(1)-C(6)	106.2(4)	C(7)-C(6)-C(5)	100.5(3)
C(2)-C(1)-Cu	71.8(2)	C(1)-C(6)-H(6)	116.3
C(6)-C(1)-Cu	115.2(3)	C(7)-C(6)-H(6)	116.3
C(2)-C(1)-H(1)	128(4)	C(5)-C(6)-H(6)	116.3
C(6)-C(1)-H(1)	124(4)	C(6)-C(7)-C(3)	95.0(3)
Cu-C(1)-H(1)	96(5)	C(6)-C(7)-H(7A)	112.7
C(1)-C(2)-C(3)	108.0(4)	C(3)-C(7)-H(7A)	112.7
C(1)-C(2)-Cu	71.7(2)	C(6)-C(7)-H(7B)	112.7
C(3)-C(2)-Cu	117.1(3)	C(3)-C(7)-H(7B)	112.7
C(1)-C(2)-H(2)	140(6)	H(7A)-C(7)-H(7B)	110.2

Symmetry transformations used to generate equivalent atoms:
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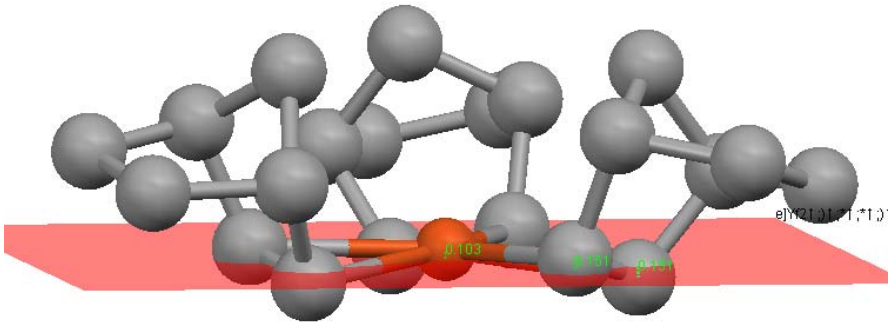

Table S3. Crystal data and structure refinement for [Ag(norbornene)$_3$][SbF$_6$], dias581s.

Identification code	dias581s	
Empirical formula	C21 H30 Ag F6 Sb	
Formula weight	626.07	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R3	
Unit cell dimensions	a = 11.5119(3) Å	α= 90°.
	b = 11.5119(3) Å	β= 90°.
	c = 14.1244(7) Å	γ = 120°.
Volume	1621.04(10) Å^3	
Z	3	
Density (calculated)	1.924 Mg/m^3	
Absorption coefficient	2.211 mm^{-1}	
F(000)	924	
Crystal size	0.29 x 0.23 x 0.21 mm^3	
Theta range for data collection	2.50 to 28.29°.	
Index ranges	-15<=h<=15, -15<=k<=15, -18<=l<=18	
Reflections collected	5260	
Independent reflections	1797 [R(int) = 0.0200]	
Completeness to theta = 28.29°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6538 and 0.5664	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1797 / 1 / 96	
Goodness-of-fit on F^2	1.143	
Final R indices [I>2sigma(I)]	R1 = 0.0175, wR2 = 0.0449	
R indices (all data)	R1 = 0.0175, wR2 = 0.0449	
Absolute structure parameter	0.08(2)	
Largest diff. peak and hole	0.972 and -0.854 e.Å^{-3}	

Table S4. Bond lengths [Å] and angles [°] for [Ag(norbornene)$_3$][SbF$_6$], dias581s.

Ag-C(2)#1	2.397(3)	C(2)-C(3)	1.513(4)
Ag-C(2)	2.397(3)	C(2)-H(2)	0.96(4)
Ag-C(2)#2	2.397(3)	C(3)-C(7)	1.537(4)
Ag-C(1)#1	2.420(3)	C(3)-C(4)	1.567(4)
Ag-C(1)	2.420(3)	C(3)-H(3)	1.0000
Ag-C(1)#2	2.420(3)	C(4)-C(5)	1.542(4)
Sb-F(2)	1.8714(19)	C(4)-H(4A)	0.9900
Sb-F(2)#3	1.8714(19)	C(4)-H(4B)	0.9900
Sb-F(2)#4	1.8714(19)	C(5)-C(6)	1.570(4)
Sb-F(1)#4	1.8769(18)	C(5)-H(5A)	0.9900
Sb-F(1)	1.8769(18)	C(5)-H(5B)	0.9900
Sb-F(1)#3	1.8769(18)	C(6)-C(7)	1.529(4)
C(1)-C(2)	1.369(4)	C(6)-H(6)	1.0000
C(1)-C(6)	1.525(4)	C(7)-H(7A)	0.9900
C(1)-H(1)	1.07(3)	C(7)-H(7B)	0.9900
C(2)#1-Ag-C(2)	119.910(8)	C(2)#1-Ag-C(1)#1	33.02(9)
C(2)#1-Ag-C(2)#2	119.910(9)	C(2)-Ag-C(1)#1	152.32(9)
C(2)-Ag-C(2)#2	119.910(8)	C(2)#2-Ag-C(1)#1	87.73(9)

C(2)#1-Ag-C(1)	87.73(9)	C(1)-C(2)-H(2)	134(3)
C(2)-Ag-C(1)	33.02(9)	C(3)-C(2)-H(2)	117(3)
C(2)#2-Ag-C(1)	152.32(10)	Ag-C(2)-H(2)	95(3)
C(1)#1-Ag-C(1)	119.35(2)	C(2)-C(3)-C(7)	101.8(2)
C(2)#1-Ag-C(1)#2	152.32(10)	C(2)-C(3)-C(4)	103.5(2)
C(2)-Ag-C(1)#2	87.73(9)	C(7)-C(3)-C(4)	99.7(2)
C(2)#2-Ag-C(1)#2	33.02(9)	C(2)-C(3)-H(3)	116.4
C(1)#1-Ag-C(1)#2	119.35(2)	C(7)-C(3)-H(3)	116.4
C(1)-Ag-C(1)#2	119.35(2)	C(4)-C(3)-H(3)	116.4
F(2)-Sb-F(2)#3	90.79(10)	C(5)-C(4)-C(3)	103.0(2)
F(2)-Sb-F(2)#4	90.79(10)	C(5)-C(4)-H(4A)	111.2
F(2)#3-Sb-F(2)#4	90.79(10)	C(3)-C(4)-H(4A)	111.2
F(2)-Sb-F(1)#4	89.94(10)	C(5)-C(4)-H(4B)	111.2
F(2)#3-Sb-F(1)#4	178.30(10)	C(3)-C(4)-H(4B)	111.2
F(2)#4-Sb-F(1)#4	90.74(10)	H(4A)-C(4)-H(4B)	109.1
F(2)-Sb-F(1)	90.74(10)	C(4)-C(5)-C(6)	103.4(2)
F(2)#3-Sb-F(1)	89.94(10)	C(4)-C(5)-H(5A)	111.1
F(2)#4-Sb-F(1)	178.30(10)	C(6)-C(5)-H(5A)	111.1
F(1)#4-Sb-F(1)	88.51(9)	C(4)-C(5)-H(5B)	111.1
F(2)-Sb-F(1)#3	178.30(10)	C(6)-C(5)-H(5B)	111.1
F(2)#3-Sb-F(1)#3	90.74(10)	H(5A)-C(5)-H(5B)	109.1
F(2)#4-Sb-F(1)#3	89.94(10)	C(1)-C(6)-C(7)	101.5(2)
F(1)#4-Sb-F(1)#3	88.51(9)	C(1)-C(6)-C(5)	104.2(2)
F(1)-Sb-F(1)#3	88.51(9)	C(7)-C(6)-C(5)	99.5(2)
C(2)-C(1)-C(6)	106.6(2)	C(1)-C(6)-H(6)	116.4
C(2)-C(1)-Ag	72.54(16)	C(7)-C(6)-H(6)	116.4
C(6)-C(1)-Ag	114.84(19)	C(5)-C(6)-H(6)	116.4
C(2)-C(1)-H(1)	130(2)	C(6)-C(7)-C(3)	94.8(2)
C(6)-C(1)-H(1)	120.0(19)	C(6)-C(7)-H(7A)	112.8
Ag-C(1)-H(1)	100.8(19)	C(3)-C(7)-H(7A)	112.8
C(1)-C(2)-C(3)	107.4(2)	C(6)-C(7)-H(7B)	112.8
C(1)-C(2)-Ag	74.44(17)	C(3)-C(7)-H(7B)	112.8
C(3)-C(2)-Ag	113.39(18)	H(7A)-C(7)-H(7B)	110.2

Symmetry transformations used to generate equivalent atoms:
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#4 -y+1,x-y+1,z

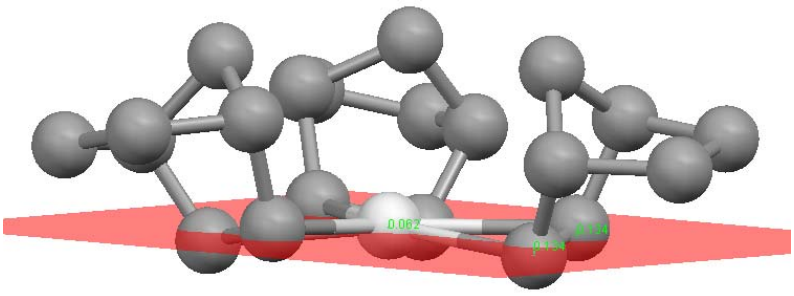

Table S5. Crystal data and structure refinement for [Au(norbornene)$_3$][SbF$_6$], dias532s.

Identification code	dias532s	
Empirical formula	C21 H30 Au F6 Sb	
Formula weight	715.17	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R3	
Unit cell dimensions	a = 11.3842(3) Å	α= 90°.
	b = 11.3842(3) Å	β= 90°.
	c = 14.1889(7) Å	γ = 120°.
Volume	1592.52(10) Å^3	
Z	3	
Density (calculated)	2.237 Mg/m^3	
Absorption coefficient	8.230 mm^{-1}	
F(000)	1020	
Crystal size	0.11 x 0.10 x 0.05 mm^3	
Theta range for data collection	2.52 to 26.47°.	
Index ranges	-14<=h<=14, -14<=k<=14, -17<=l<=17	
Reflections collected	4623	
Independent reflections	1475 [R(int) = 0.0174]	
Completeness to theta = 26.47°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6837 and 0.4646	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1475 / 1 / 96	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0156, wR2 = 0.0395	
R indices (all data)	R1 = 0.0156, wR2 = 0.0395	
Absolute structure parameter	0.003(4)	
Largest diff. peak and hole	0.712 and -0.366 e.Å^{-3}	

Table S6. Bond lengths [Å] and angles [°] for [Au(norbornene)$_3$][SbF$_6$], dias532s.

Au-C(2)#1	2.281(3)	C(2)-C(3)	1.522(5)
Au-C(2)	2.281(3)	C(2)-H(2)	0.92(5)
Au-C(2)#2	2.281(3)	C(3)-C(7)	1.539(5)
Au-C(1)	2.302(4)	C(3)-C(4)	1.554(5)
Au-C(1)#1	2.302(4)	C(3)-H(3)	1.0000
Au-C(1)#2	2.302(4)	C(4)-C(5)	1.551(5)
Sb-F(1)#3	1.872(3)	C(4)-H(4A)	0.9900
Sb-F(1)	1.872(3)	C(4)-H(4B)	0.9900
Sb-F(1)#4	1.872(3)	C(5)-C(6)	1.566(5)
Sb-F(2)	1.878(2)	C(5)-H(5A)	0.9900
Sb-F(2)#3	1.878(2)	C(5)-H(5B)	0.9900
Sb-F(2)#4	1.878(2)	C(6)-C(7)	1.539(5)
C(1)-C(2)	1.378(5)	C(6)-H(6)	1.0000
C(1)-C(6)	1.509(5)	C(7)-H(7A)	0.9900
C(1)-H(1)	0.96(5)	C(7)-H(7B)	0.9900
C(2)#1-Au-C(2)	119.980(4)	C(2)#1-Au-C(1)	85.55(13)
C(2)#1-Au-C(2)#2	119.980(5)	C(2)-Au-C(1)	34.99(13)
C(2)-Au-C(2)#2	119.980(5)	C(2)#2-Au-C(1)	154.24(13)

C(2)#1-Au-C(1)#1	34.99(13)	C(1)-C(2)-H(2)	129(3)
C(2)-Au-C(1)#1	154.24(13)	C(3)-C(2)-H(2)	119(3)
C(2)#2-Au-C(1)#1	85.55(13)	Au-C(2)-H(2)	105(3)
C(1)-Au-C(1)#1	119.25(3)	C(2)-C(3)-C(7)	102.0(3)
C(2)#1-Au-C(1)#2	154.24(13)	C(2)-C(3)-C(4)	103.4(3)
C(2)-Au-C(1)#2	85.55(13)	C(7)-C(3)-C(4)	100.1(3)
C(2)#2-Au-C(1)#2	34.99(13)	C(2)-C(3)-H(3)	116.3
C(1)-Au-C(1)#2	119.25(3)	C(7)-C(3)-H(3)	116.3
C(1)#1-Au-C(1)#2	119.25(3)	C(4)-C(3)-H(3)	116.3
F(1)#3-Sb-F(1)	90.39(12)	C(5)-C(4)-C(3)	103.0(3)
F(1)#3-Sb-F(1)#4	90.39(12)	C(5)-C(4)-H(4A)	111.2
F(1)-Sb-F(1)#4	90.39(12)	C(3)-C(4)-H(4A)	111.2
F(1)#3-Sb-F(2)	178.80(12)	C(5)-C(4)-H(4B)	111.2
F(1)-Sb-F(2)	89.81(12)	C(3)-C(4)-H(4B)	111.2
F(1)#4-Sb-F(2)	90.79(12)	H(4A)-C(4)-H(4B)	109.1
F(1)#3-Sb-F(2)#3	89.81(12)	C(4)-C(5)-C(6)	103.5(3)
F(1)-Sb-F(2)#3	90.79(12)	C(4)-C(5)-H(5A)	111.1
F(1)#4-Sb-F(2)#3	178.80(11)	C(6)-C(5)-H(5A)	111.1
F(2)-Sb-F(2)#3	89.00(11)	C(4)-C(5)-H(5B)	111.1
F(1)#3-Sb-F(2)#4	90.79(12)	C(6)-C(5)-H(5B)	111.1
F(1)-Sb-F(2)#4	178.80(11)	H(5A)-C(5)-H(5B)	109.0
F(1)#4-Sb-F(2)#4	89.81(12)	C(1)-C(6)-C(7)	101.6(3)
F(2)-Sb-F(2)#4	89.00(11)	C(1)-C(6)-C(5)	103.4(3)
F(2)#3-Sb-F(2)#4	89.00(11)	C(7)-C(6)-C(5)	99.4(3)
C(2)-C(1)-C(6)	107.6(3)	C(1)-C(6)-H(6)	116.6
C(2)-C(1)-Au	71.7(2)	C(7)-C(6)-H(6)	116.6
C(6)-C(1)-Au	116.7(2)	C(5)-C(6)-H(6)	116.6
C(2)-C(1)-H(1)	130(3)	C(3)-C(7)-C(6)	94.8(3)
C(6)-C(1)-H(1)	116(3)	C(3)-C(7)-H(7A)	112.8
Au-C(1)-H(1)	106(3)	C(6)-C(7)-H(7A)	112.8
C(1)-C(2)-C(3)	106.4(3)	C(3)-C(7)-H(7B)	112.8
C(1)-C(2)-Au	73.3(2)	C(6)-C(7)-H(7B)	112.8
C(3)-C(2)-Au	115.3(2)	H(7A)-C(7)-H(7B)	110.2

Symmetry transformations used to generate equivalent atoms:
#1 -y+1,x-y,z #2 -x+y+1,-x+1,z #3 -x+y+2,-x+1,z
#4 -y+1,x-y-1,z