Electronic Supplementary Material (ESI) for ChemComm.

Gold(I) ethylene complexes supported by electron-rich scorpionates

Jiang Wu,[†] Anurag Noonikara-Poyil,[†] Alvaro Muñoz-Castro,[‡] and H. V. Rasika Dias[†,*]

[†]Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, Texas 76019. E-mail: dias@uta.edu

[‡]Grupo de Química Inorgánica y Materiales Moleculares, Facultad de Ingeniería, Universidad Autonoma de Chile, El Llano Subercaseaux 2801, Santiago, Chile.

Supporting information

Table S1. Gold bound ethylene C=C distances (Å) and Au-C distances (Å) and ^{13}C chemical shift values of ethylene carbons (ppm) for structurally characterized compounds in the literature

Compound	C=C	Au-C	Au-C	^{13}C of $H_2C=$	Ref
Mono-ethylene complexes					
$[PhB(3\text{-}(C_2F_5)Pz)_3]Au(C_2H_4)$	1.366	2.105	2.090	58.9 (C_6D_{12})	[1]
$[HB(3,5\text{-}(CF_3)_2Pz)_3]Au(C_2H_4)$	1.380	2.096	2.109	63.7 ($CDCl_3$)	[2]
$[HB(3\text{-}(CF_3),5\text{-}(Ph)Pz)_3]Au(C_2H_4)$	1.387	2.095	2.093	59.3 ($CDCl_3$)	[2]
$[HB(3\text{-}(CF_3),5\text{-}(Me)Pz)_3]Au(C_2H_4)$	Structurally confirmed but ethylene moiety is disordered			58.3 ($CDCl_3$)	[3]
$[(5,5'\text{-}F_2\text{-}2,2'\text{-bipy})Au(C_2H_4)][N(SO_2CF_3)_2]$	*1.397*	*2.100*	*2.095*	60.6	[4]
$[(2,9\text{-}(n\text{-}Bu)_2\text{-}1,10\text{-phen})Au(C_2H_4)][N(SO_2CF_3)_2]$**	1.399	2.092	2.087	63.8	[5]
$[[N\{(C_3F_7)C(2,6\text{-}Cl_2C_6H_3)N\}_2]Au(C_2H_4)$	1.405	2.098	2.089	59.1	[6]
$[1,4\text{-}(2,6\text{-}Cl_2Ph(napth)\text{-}2,3\text{-}Me_2\text{-}butanediimine)Au(C_2H_4)][SbF_6]$	1.455	2.094	2.119	65.4	[7]
$[HB(3,5\text{-}(Ph)_3Pz)_3]Au(C_2H_4)$	1.413	2.091	2.194	55.3 (CD_2Cl_2)	This work
$[HB(3,5\text{-}(t\text{-}Bu)_3Pz)_3]Au(C_2H_4)$	1.410	2.102	2.205	56.9 (C_7D_8)	This work
Tris(ethylene) complexes					
*$[Au(C_2H_4)_3][Al\{OC(CF_3)_3\}_4]$***	*1.346*	*2.304*	*2.308*	104	[8]
*$[Au(C_2H_4)_3][SbF_6]$***	*1.364*	*2.267*	*2.269*	92.7	[9]

***X-ray crystallographic parameters of these molecules are the average of several ethylene moieties in the asymmetric unit.*

^{13}C resonance of free ethylene[10]= 123.1 ($CDCl_3$); 123.2 (CD_2Cl_2); 122.9 (toluene-d_8).

The C=C bond length of free ethylene = 1.3305 Å.[11]

Experimental section:

All manipulations were carried out under an atmosphere of purified nitrogen using standard Schlenk techniques or in a vacuum atmosphere single-station drybox equipped with a -25 °C refrigerator. Solvents were purchased from commercial sources, purified prior to use. NMR spectra were recorded on a JEOL Eclipse 500, JEOL Eclipse 400, and JEOL Eclipse 300 spectrometer (^{1}H, 500.16 MHz, 399.78 MHz, and 300.53 MHz; ^{13}C, 125.78 MHz, 100.52 MHz, and 75.59 MHz). ^{1}H and ^{13}C NMR spectra are referenced to the solvent peak (^{1}H; CD_2Cl_2 δ 5.32, C_6D_{12} δ 1.38, toluene-d_8 δ 2.08 ^{13}C; CD_2Cl_2 δ 53.8, toluene-d_8 δ 137.8). The NMR samples were prepared inside the drybox to prevent decomposition. To perform the low-temperature NMR, the samples were transferred to a -78 ºC bath (acetone and dry ice) and taken to NMR spectrometer and loaded at -20 ºC. Ethylene gas was purchased from Matheson. The [HB(3,5-(*t*-Bu)$_2$Pz)$_3$]K[12] and [HB(3,5-(Ph)$_2$Pz)$_3$]K[13] were synthesized using reported procedures. Elemental analyses were performed using a Perkin Elmer Series II CHNS/O analyzer. Moisture and light must be avoided strictly to prevent decomposition.

[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$): Solid [HB(3,5-(*t*-Bu)$_2$Pz)$_3$]K (0.20 g, 0.34mmol) and gold(I) chloride (0.079 g, 0.34mmol) were placed in a Schlenk flask (protected from light with some aluminum foil). To this mixture, 20 mL of hexane saturated with ethylene at 0 °C was added, and the solution was stirred for 20 minutes. Ethylene gas was gently bubbled through the solution about 2-3 times (30 sec each time) during this period. The yellow color of the solution turned slowly dark and an off-white precipitate was formed. The mixture was filtered under N_2 through a bed of Celite, and the filtrate was concentrated under reduced pressure to obtain [HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$) as a colorless solid (0.21 g, 77%). X-ray quality crystals were obtained from a hexane solution saturated with ethylene at -20 °C. These samples are difficult to handle at room temperature due to decomposition, which is particularly notable in solutions. Anal. Calc. for $C_{35}H_{62}AuBN_6$: C, 54.26; H, 8.07; N, 10.85; Found: C, 53.89; H, 8.31; N, 10.50. ^{1}H NMR (C_6D_{12}, 298 K): δ 1.18 (s, 27H, *t-Bu*), 1.22 (s, 27H, *t-Bu*), 3.01 (m, 4H, C$_2$*H$_4$*), 5.91 (s, 3H, Pz*H*); ^{1}H NMR (Toluene-*d$_8$*, 253 K): δ 1.34 (s, 27H, *t-Bu*), 1.37 (s, 27H, *t-Bu*), 3.00 (m, 4H, C$_2$*H$_4$*), 6.15 (s, 3H, Pz*H*); bonded ethylene doesn't exchange with added free ethylene in both solvents. ^{13}C{^{1}H} NMR (Toluene-*d$_8$*, 253 K): 31.1 (s), 31.4 (s), 32.4 (s), 32.6 (s), 33.1 (s), 56.9 (s, *C$_2$H$_4$*), 101.9 (s, PzC-4), 158.0 (s, PzC-3/C-5), 161.0 (s, PzC-3/C-5).

[HB(3,5-(Ph)$_2$Pz)$_3$]Au(C$_2$H$_4$): Solid [HB(3,5-(Ph)$_2$Pz)$_3$]K (0.20 g, 0.28 mmol) and gold(I) chloride (0.065 g, 0.28 mmol) were placed in a Schlenk flask. To this mixture, 8 mL of CH_2Cl_2 saturated with ethylene at -18 °C was added, and the solution was stirred for 40 minutes. Ethylene gas was gently bubbled through the solution about 2-3 times (30 sec each time) during this period. The yellow color of the solution turned slowly pale and

cleared in 10 minutes. The mixture was filtered under N_2 through a bed of Celite, and the filtrate was concentrated under reduced pressure to obtain [HB(3,5-$(Ph)_2Pz)_3$]Au(C_2H_4)•CH_2Cl_2 as a pale-yellow solid (0.17 g, 62%). X-ray quality crystals were obtained from a CH_2Cl_2/hexane solution saturated with ethylene at -20 °C. Anal. Calc. for $C_{47}H_{38}AuBN_6$•1.3(CH_2Cl_2): C, 57.72; H, 4.07; N, 8.36; Found: C, 57.74; H, 4.58; N, 8.30 (these molecules are temperature sensitive for prolong handling or drying). ^{1}H NMR (CD_2Cl_2, 253 K): 2.61 (s, 4H, C_2H_4), 6.51 (s, 3H, Pz*H*), 6.99-7.10 (m, 12H, Ph-*H*), 7.19-7.23 (m, 3H, Ph-*H*), 7.32-7.42 (m, 10H, Ph-*H*), 7.64-7.66 (m, 5H, Ph-*H*), ; bonded ethylene doesn't exchange with added free ethylene; ^{13}C{^{1}H} NMR (CD_2Cl_2, 253 K): 55.3 (s, C_2H_4), 105.3 (s, PzC-4), 125.6 (s), 127.7 (s), 127.8 (s), 128.1 (s), 128.3 (s), 129.6 (s), 132.1 (s), 133.8 (s),151.0 (s, PzC-3/C-5), 152.9 (s, PzC-3/C-5).

^{1}H and ^{13}C NMR spectra of Metal complexes

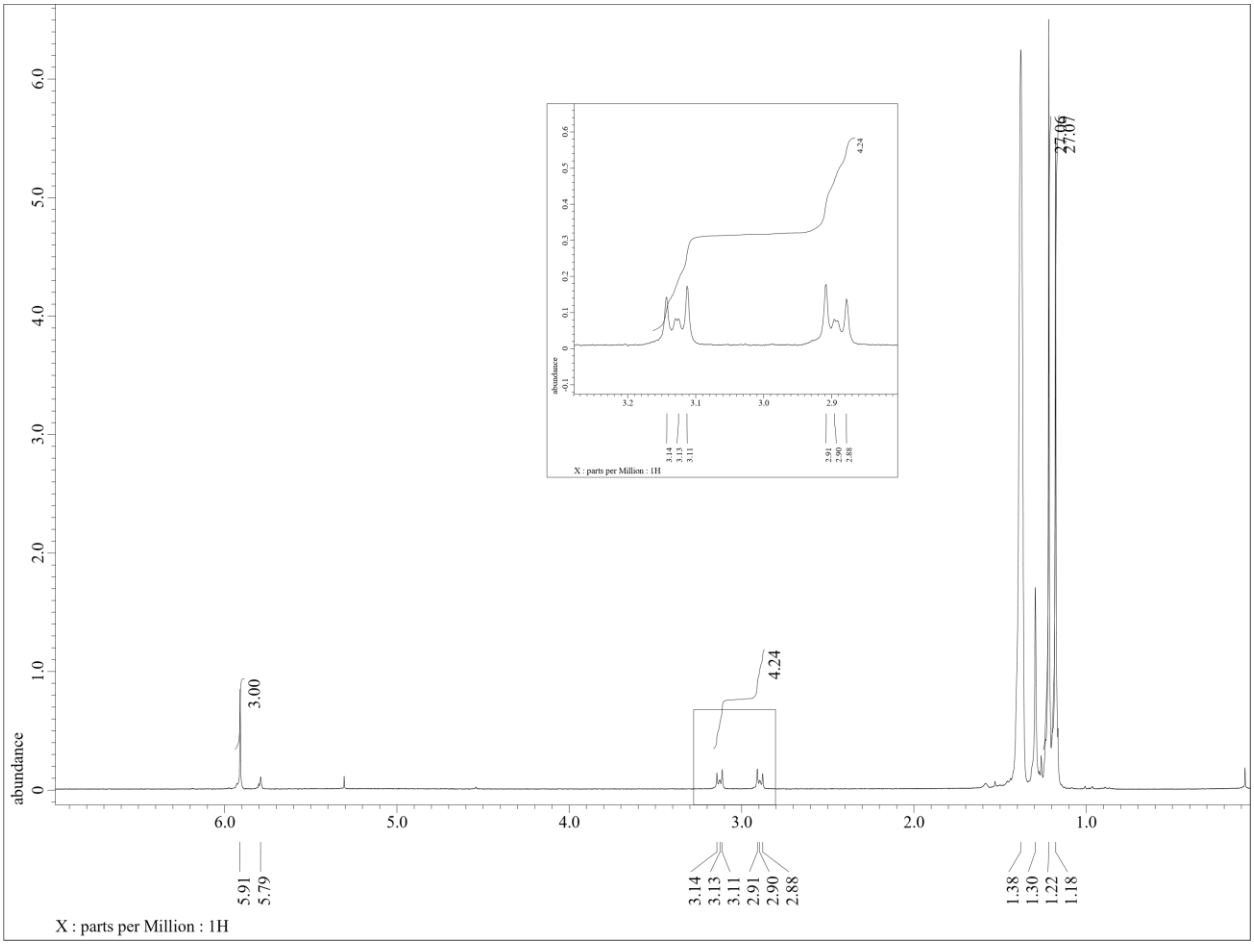

Figure S1. ^{1}H NMR spectrum of **[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)** at 298 K in C_6D_{12}. The small peaks at 5.79 and 1.30 are from the decomposed product.

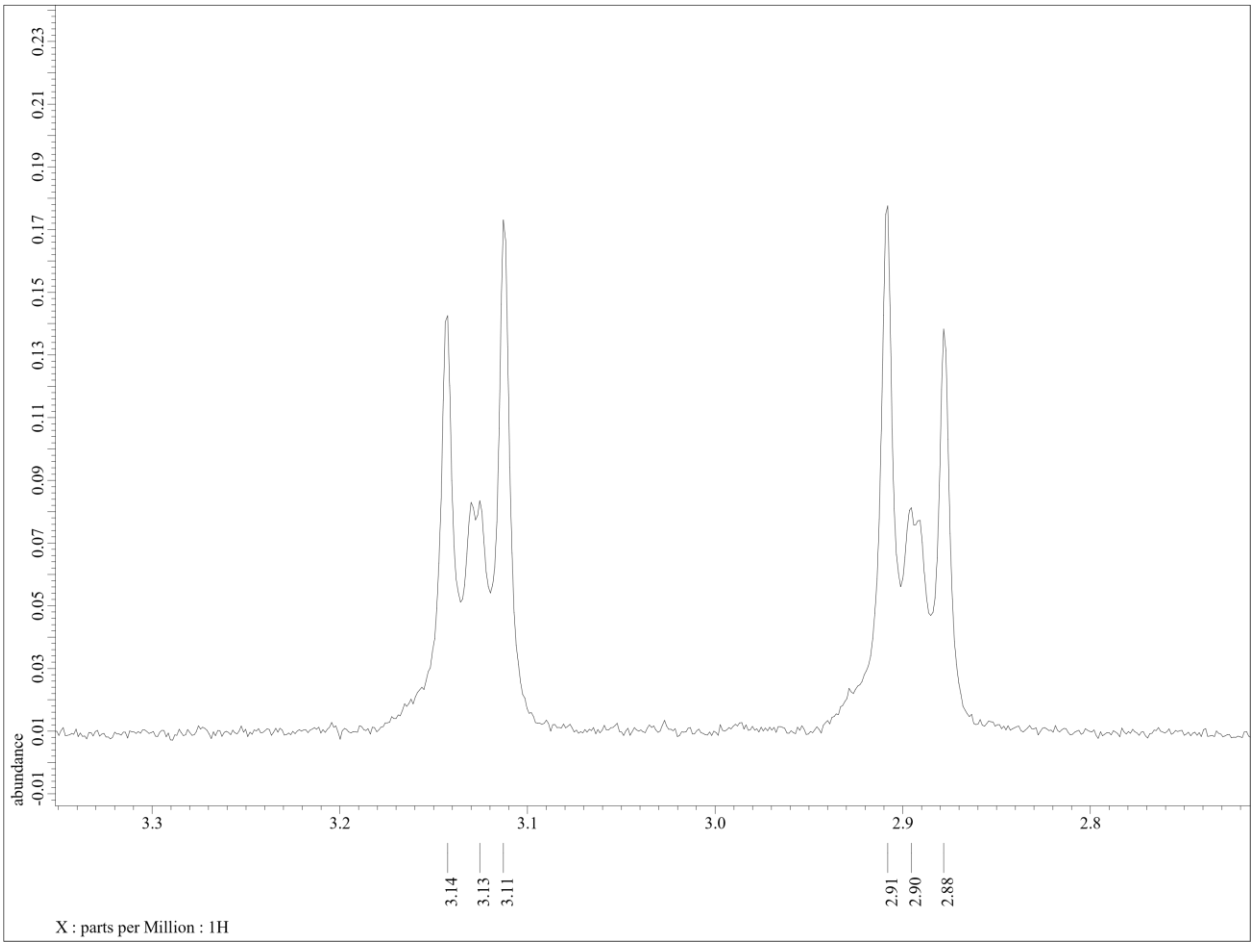

Figure S2. ^{1}H NMR spectrum of **[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)** showing AA'BB' pattern of ethylene protons at 298 K in C_6D_{12}.

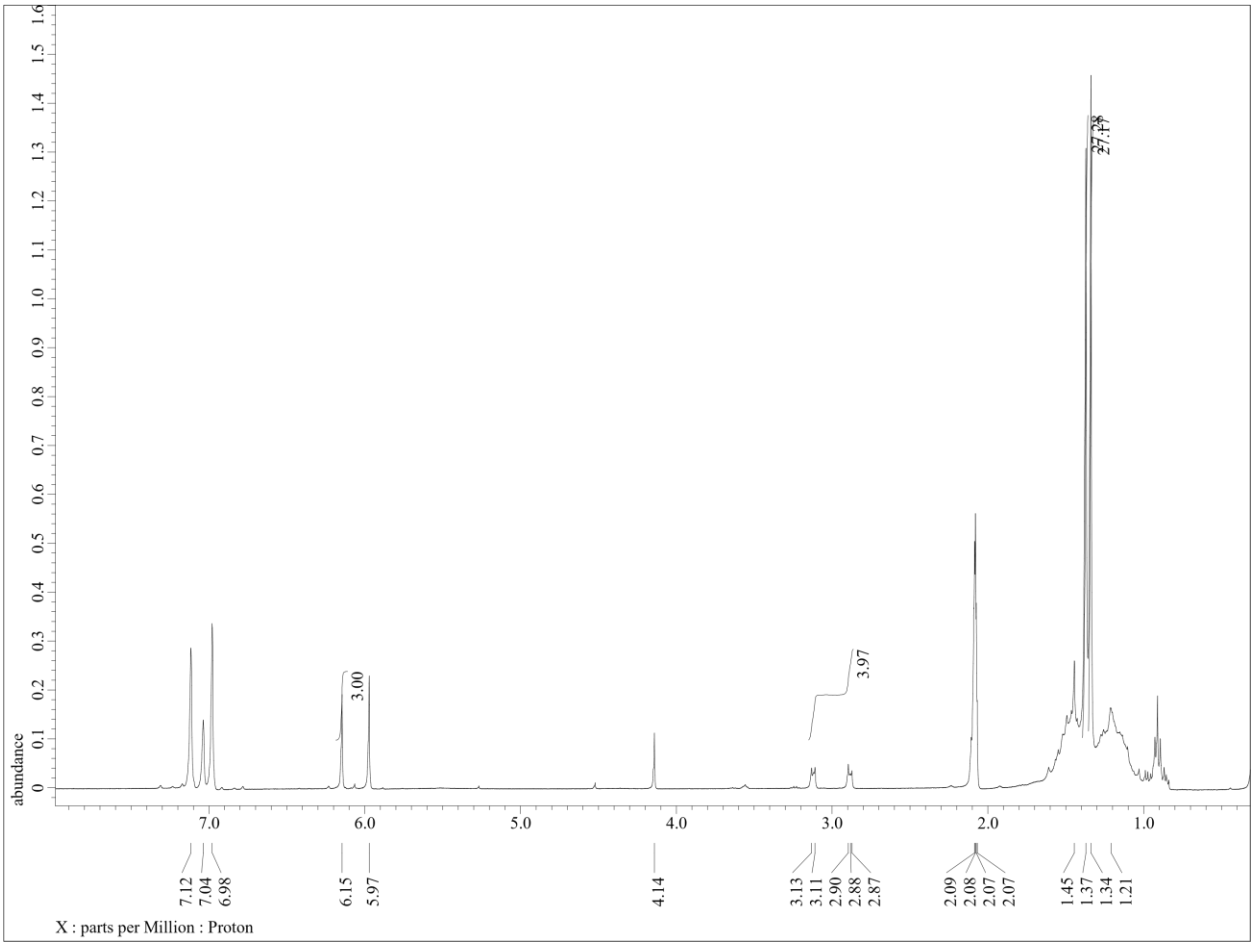

Figure S3. ^{1}H NMR spectrum of **[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)** at 253 K in toluene-d_8. The compound slowly decomposes at room temperature in solution. It is possible to identify the resonances resulting from decomposition products by monitoring the spectrum with time. The peak at 5.97, 4.14, 1.45 and 1.21 are from the decomposed product.

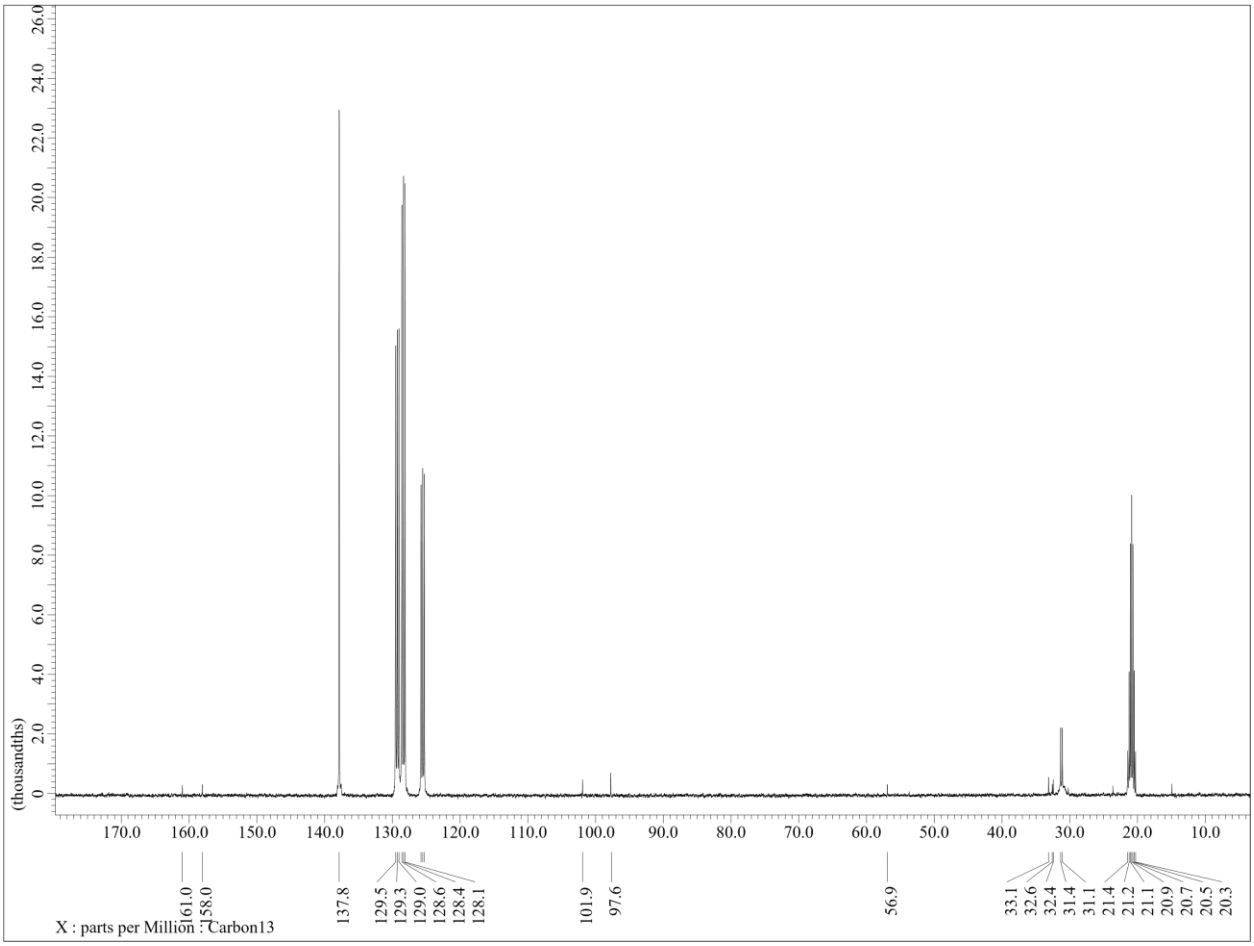

Figure S4. ^{13}C NMR spectrum of **[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)** at 253 K in toluene-d_8. The peak at 97.6 is from a product resulting from decomposition.

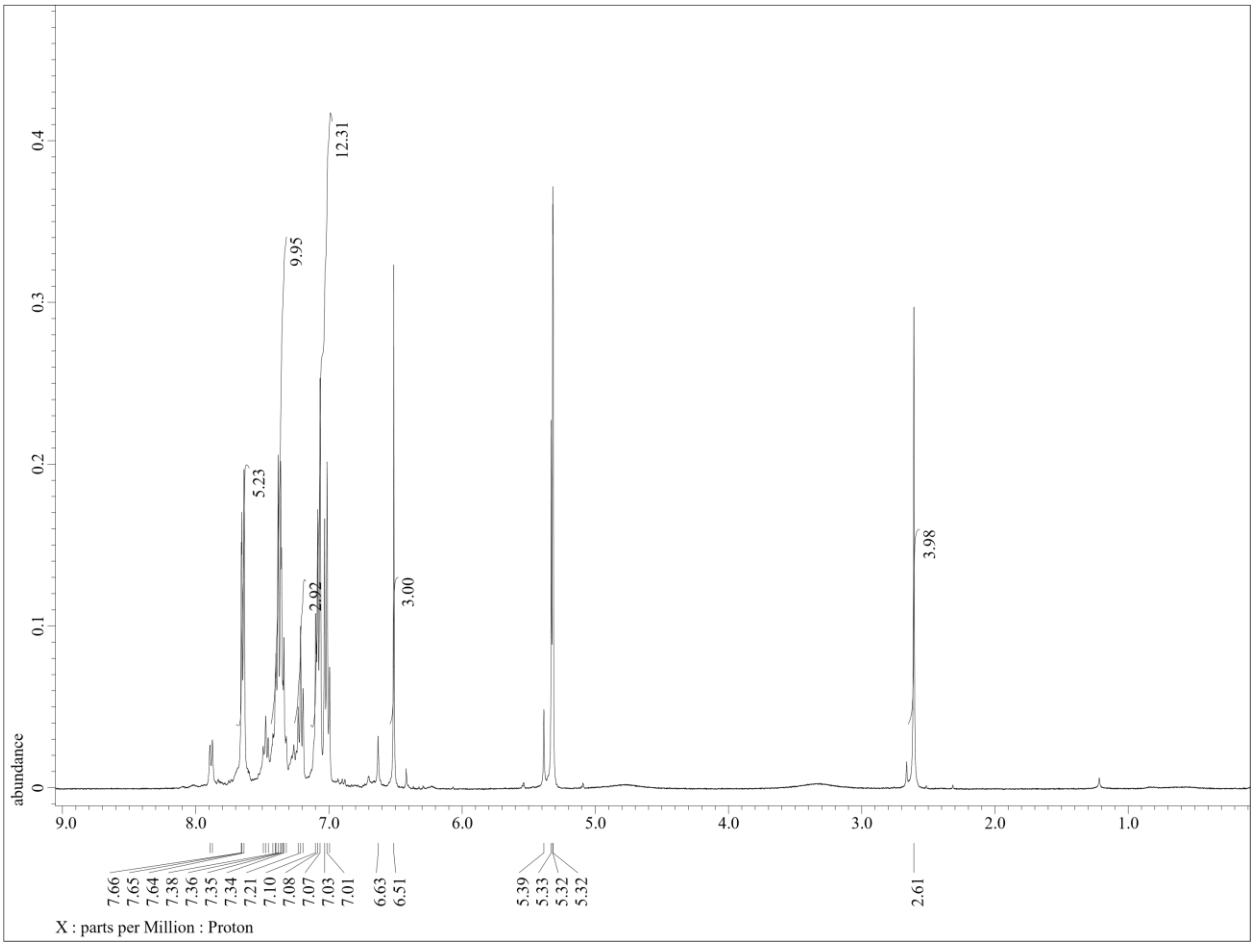

Figure S5. ^{1}H NMR spectrum of **[HB(3,5-(Ph)$_2$Pz)$_3$]Au(C$_2$H$_4$)** at 253 K in CD_2Cl_2. The compound slowly decomposes at room temperature in solution. The peak at 7.89-7.87, 7.49-7.45, and 6.63 are from product/s resulting from decomposition. It is possible to identify the resonances resulting from decomposition products by monitoring the spectrum with time.

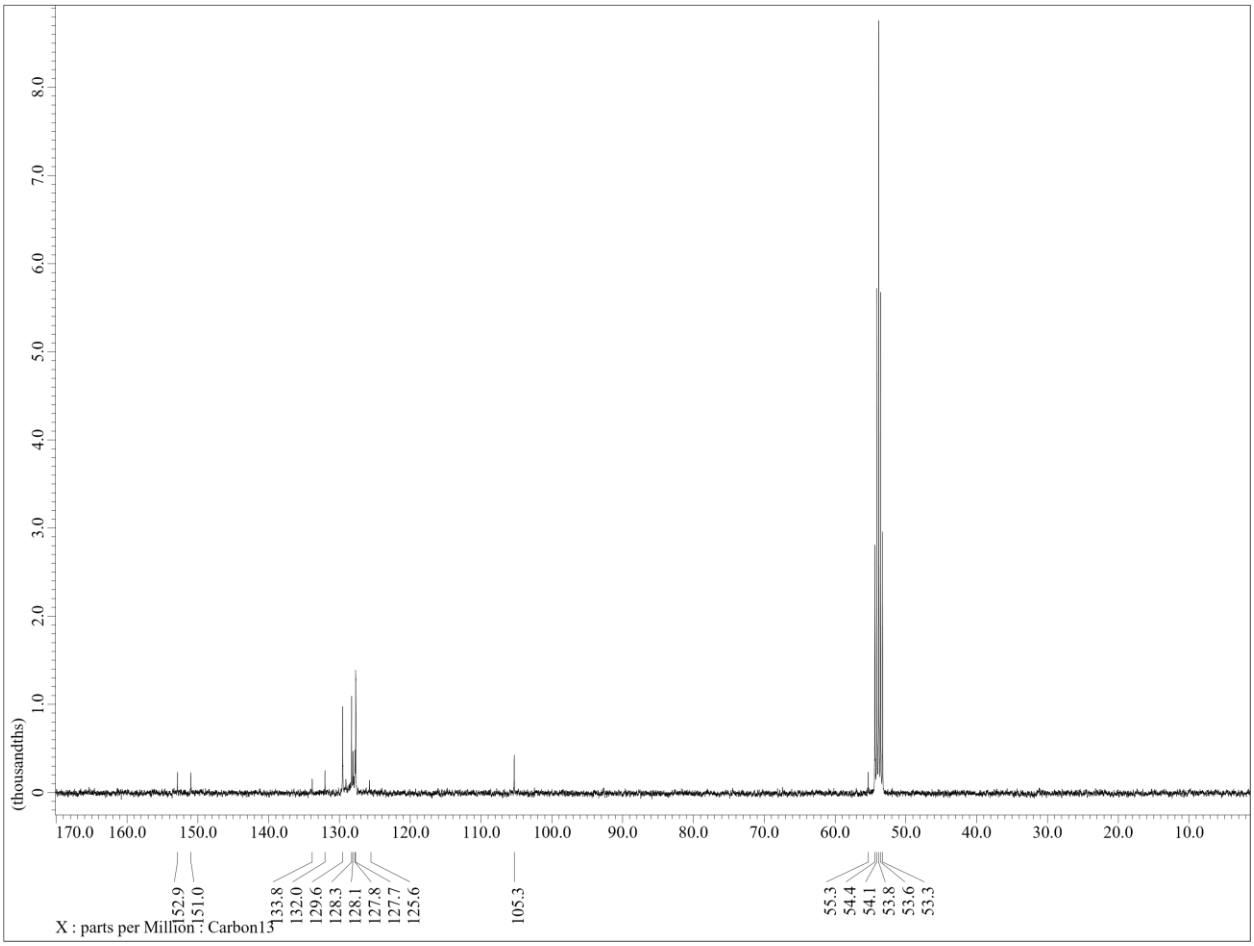

Figure S6. ^{13}C NMR spectrum of **[HB(3,5-(Ph)$_2$Pz)$_3$]Au(C$_2$H$_4$)** at 253 K in CD_2Cl_2.

X-ray crystallographic data:

A suitable crystal covered with a layer of hydrocarbon/paratone-N oil was selected and mounted on a Cryo-loop, and immediately placed in the low-temperature nitrogen stream. The X-ray intensity data for [HB(3,5-$(Ph)_2Pz)_3$]Au(C_2H_4) and [HB(3,5-(*t*-$Bu)_2Pz)_3$]Au(C_2H_4) were measured at 100(2) K on a SMART APEX II CCD area detector system equipped with an Oxford Cryosystems 700 series cooler, a graphite monochromator, and a Mo Kα fine-focus sealed tube (λ = 0.71073 Å). Intensity data were processed using the Bruker Apex2 program suite. Initial atomic positions were located by direct methods using SHELXT, and the structures of the compounds were refined by the least-squares method using SHELXL.[14] Absorption corrections were applied by using SADABS. All the non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed at calculated positions and refined using a riding model. X-ray structural figures were generated using Olex2.[15] The [HB(3,5-$(Ph)_2Pz)_3$]Au(C_2H_4) crystallizes with a CH_2Cl_2 molecule in the asymmetric unit. Further details are given in Table S2 and S6. The CCDC 2045804-2045805 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).

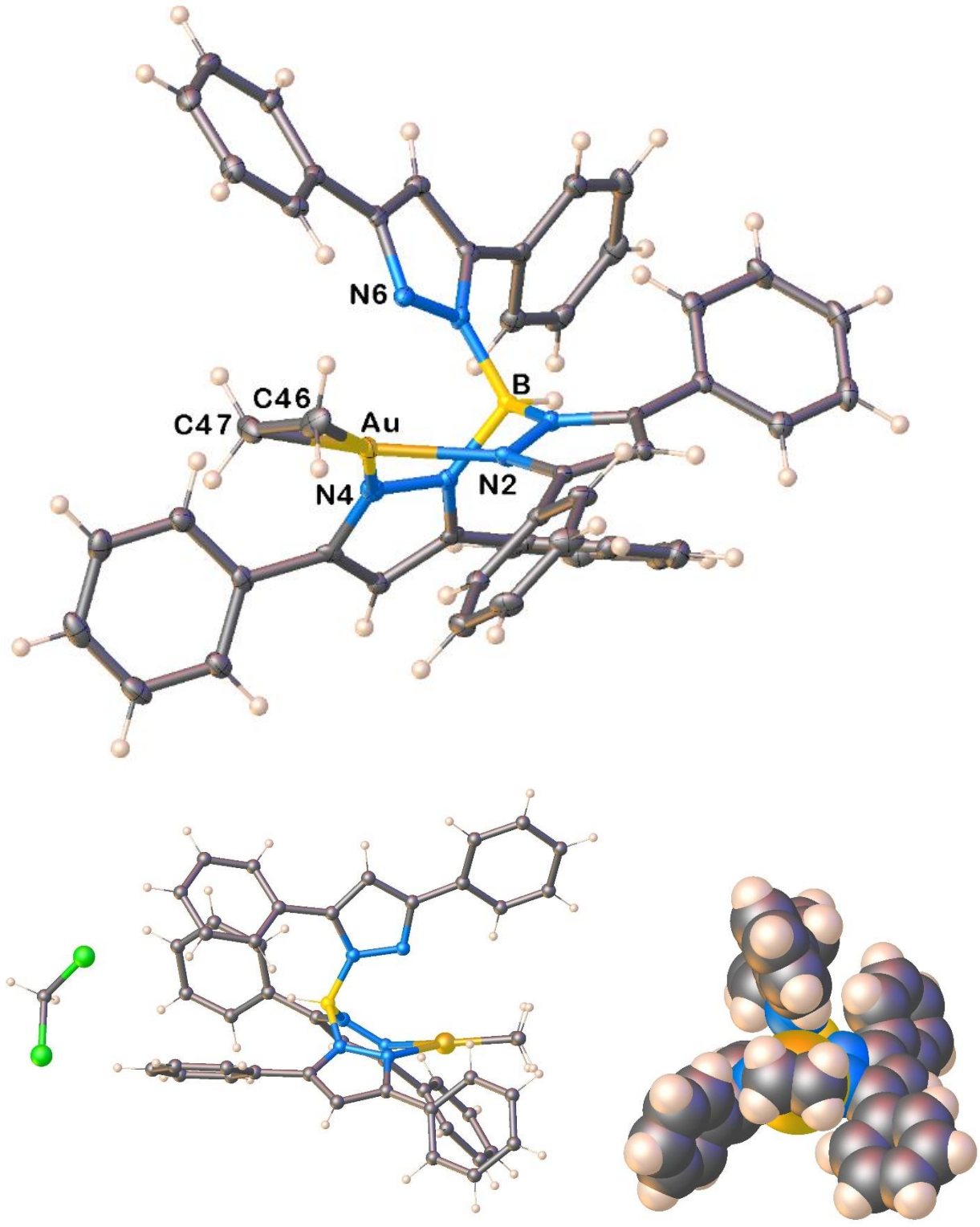

Figure S7. Three view of for **[HB(3,5-(Ph)$_2$Pz)$_3$]Au(C$_2$H$_4$)•CH$_2$Cl$_2$** (dichloromethane has been omitted from two figures for clarity)

Table S2. Crystal data and structure refinement for $[HB(3,5\text{-}(Ph)_2Pz)_3]Au(C_2H_4)\bullet CH_2Cl_2$.

Identification code	Dias528
Empirical formula	$C_{48}H_{40}AuBCl_2N_6$
Formula weight	979.53
Temperature/K	100.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	13.1586(7)
b/Å	17.0373(10)
c/Å	18.2948(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4101.5(4)
Z	4
ρ_{calc}g/cm^3	1.586
μ/mm^{-1}	3.760
F(000)	1952.0
Crystal size/mm^3	0.18 × 0.113 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.452 to 56.54
Index ranges	$-17 \le h \le 17$, $-22 \le k \le 22$, $-24 \le l \le 24$
Reflections collected	36358
Independent reflections	10115 [R_{int} = 0.0368, R_{sigma} = 0.0496]
Data/restraints/parameters	10115/0/523
Goodness-of-fit on F^2	1.016
Final R indexes [I>=2σ (I)]	R_1 = 0.0242, wR_2 = 0.0537
Final R indexes [all data]	R_1 = 0.0262, wR_2 = 0.0545
Largest diff. peak/hole / e Å^{-3}	1.49/-0.41

Table S3. Bond Lengths for $[HB(3,5\text{-}(Ph)_2Pz)_3]Au(C_2H_4)\bullet CH_2Cl_2$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au	N2	2.177(4)	C17	C18	1.372(6)
Au	N4	2.211(3)	C18	C25	1.488(6)
Au	C46	2.100(5)	C19	C20	1.400(6)
Au	C47	2.082(4)	C19	C24	1.401(6)
N1	N2	1.372(5)	C20	C21	1.389(6)
N1	B	1.550(6)	C21	C22	1.376(7)
N1	C3	1.365(5)	C22	C23	1.394(7)
N2	C1	1.351(5)	C23	C24	1.391(6)

N3	N4	1.361(5)	C25	C26	1.389(6)
N3	B	1.564(5)	C25	C30	1.395(6)
N3	C18	1.351(5)	C26	C27	1.395(7)
N4	C16	1.353(5)	C27	C28	1.378(7)
N5	N6	1.368(5)	C28	C29	1.380(7)
N5	B	1.536(6)	C29	C30	1.398(7)
N5	C33	1.365(6)	C31	C32	1.406(6)
N6	C31	1.336(5)	C31	C34	1.467(6)
C1	C2	1.391(6)	C32	C33	1.377(6)
C1	C4	1.473(6)	C33	C40	1.485(6)
C2	C3	1.371(6)	C34	C35	1.400(6)
C3	C10	1.481(6)	C34	C39	1.401(6)
C4	C5	1.394(6)	C35	C36	1.379(7)
C4	C9	1.402(6)	C36	C37	1.385(6)
C5	C6	1.388(6)	C37	C38	1.389(7)
C6	C7	1.385(6)	C38	C39	1.386(7)
C7	C8	1.385(7)	C40	C41	1.391(6)
C8	C9	1.383(6)	C40	C45	1.398(6)
C10	C11	1.391(6)	C41	C42	1.394(6)
C10	C15	1.396(6)	C42	C43	1.382(7)
C11	C12	1.396(6)	C43	C44	1.376(7)
C12	C13	1.383(7)	C44	C45	1.388(7)
C13	C14	1.398(7)	C46	C47	1.413(7)
C14	C15	1.376(6)	C48	Cl1	1.772(5)
C16	C17	1.394(6)	C48	Cl2	1.752(5)
C16	C19	1.475(6)			

Table S4. Bond Angles for [HB(3,5-(Ph)$_2$Pz)$_3$]Au(C$_2$H$_4$)•CH$_2$Cl$_2$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Au	N4	86.12(13)	N4	C16	C19	122.6(4)
C46	Au	N2	114.40(17)	C17	C16	C19	128.5(4)
C46	Au	N4	158.71(17)	C18	C17	C16	106.2(4)
C47	Au	N2	153.88(16)	N3	C18	C17	108.3(4)
C47	Au	N4	119.91(16)	N3	C18	C25	123.8(4)
C47	Au	C46	39.49(18)	C17	C18	C25	127.9(4)
N2	N1	B	121.0(3)	C20	C19	C16	121.8(4)
C3	N1	N2	109.2(3)	C20	C19	C24	118.6(4)
C3	N1	B	129.2(4)	C24	C19	C16	119.5(4)
N1	N2	Au	120.3(3)	C21	C20	C19	120.5(4)
C1	N2	Au	131.2(3)	C22	C21	C20	120.3(5)

C1	N2	N1	106.7(3)	C21	C22	C23	120.2(5)
N4	N3	B	121.1(3)	C24	C23	C22	119.8(4)
C18	N3	N4	109.4(3)	C23	C24	C19	120.5(4)
C18	N3	B	128.9(4)	C26	C25	C18	121.8(4)
N3	N4	Au	117.1(3)	C26	C25	C30	119.3(4)
C16	N4	Au	129.4(3)	C30	C25	C18	118.9(4)
C16	N4	N3	107.3(3)	C25	C26	C27	120.1(5)
N6	N5	B	121.9(3)	C28	C27	C26	119.9(5)
C33	N5	N6	109.8(4)	C27	C28	C29	121.0(5)
C33	N5	B	128.1(4)	C28	C29	C30	119.3(5)
C31	N6	N5	106.6(4)	C25	C30	C29	120.4(5)
N1	B	N3	108.1(3)	N6	C31	C32	110.5(4)
N5	B	N1	112.1(3)	N6	C31	C34	121.1(4)
N5	B	N3	111.4(3)	C32	C31	C34	128.4(4)
N2	C1	C2	109.8(4)	C33	C32	C31	105.2(4)
N2	C1	C4	122.6(4)	N5	C33	C32	107.9(4)
C2	C1	C4	127.6(4)	N5	C33	C40	124.7(4)
C3	C2	C1	106.2(4)	C32	C33	C40	127.3(4)
N1	C3	C2	108.1(4)	C35	C34	C31	120.7(4)
N1	C3	C10	124.2(4)	C35	C34	C39	117.9(4)
C2	C3	C10	127.7(4)	C39	C34	C31	121.4(4)
C5	C4	C1	122.0(4)	C36	C35	C34	120.9(4)
C5	C4	C9	118.5(4)	C35	C36	C37	120.7(4)
C9	C4	C1	119.2(4)	C36	C37	C38	119.3(4)
C6	C5	C4	120.6(4)	C39	C38	C37	120.2(4)
C7	C6	C5	120.2(4)	C38	C39	C34	120.9(4)
C8	C7	C6	119.8(4)	C41	C40	C33	121.7(4)
C9	C8	C7	120.3(4)	C41	C40	C45	119.0(4)
C8	C9	C4	120.6(4)	C45	C40	C33	119.1(4)
C11	C10	C3	122.2(4)	C40	C41	C42	120.0(4)
C11	C10	C15	118.9(4)	C43	C42	C41	120.3(5)
C15	C10	C3	118.8(4)	C44	C43	C42	120.0(4)
C10	C11	C12	120.0(4)	C43	C44	C45	120.2(4)
C13	C12	C11	120.4(4)	C44	C45	C40	120.4(5)
C12	C13	C14	119.8(4)	C47	C46	Au	69.6(3)
C15	C14	C13	119.5(4)	C46	C47	Au	70.9(3)
C14	C15	C10	121.4(4)	Cl2	C48	Cl1	112.1(3)
N4	C16	C17	108.8(4)				

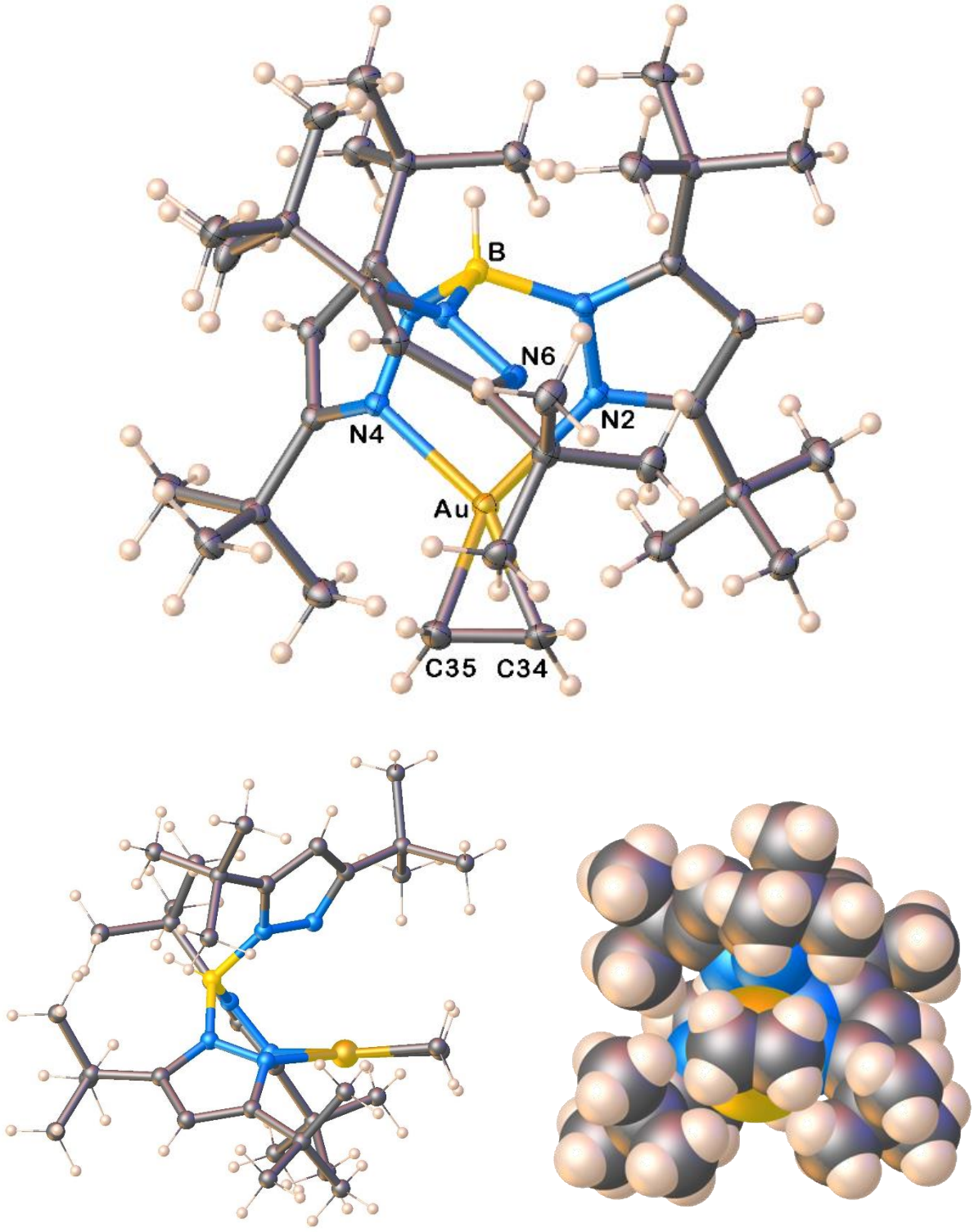

Figure S8. Three view of for **[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)**.

Table S5. Crystal data and structure refinement for [HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$).

Identification code	Dias482
Empirical formula	$C_{35}H_{62}AuBN_6$
Formula weight	774.68
Temperature/K	100.15
Crystal system	triclinic
Space group	P-1
a/Å	10.485(2)
b/Å	10.623(2)
c/Å	18.198(4)
α/°	104.587(3)
β/°	92.945(3)
γ/°	102.963(3)
Volume/Å^3	1899.2(7)
Z	2
ρ_{calc}g/cm^3	1.355
μ/mm^{-1}	3.903
F(000)	796.0
Crystal size/mm^3	0.19 × 0.14 × 0.06
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.086 to 53.46
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -22 ≤ l ≤ 23
Reflections collected	16099
Independent reflections	7977 [R_{int} = 0.0204, R_{sigma} = 0.0263]
Data/restraints/parameters	7977/0/406
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0297, wR_2 = 0.0792
Final R indexes [all data]	R_1 = 0.0308, wR_2 = 0.0800
Largest diff. peak/hole / e Å^{-3}	3.55/-1.62

Table S6. Bond Lengths for [HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au	N2	2.230(3)	C8	C10	1.541(5)
Au	N4	2.180(3)	C8	C11	1.538(4)
Au	C34	2.112(3)	C12	C13	1.393(4)
Au	C35	2.092(3)	C12	C15	1.515(4)
N1	N2	1.378(4)	C13	C14	1.388(4)
N1	C3	1.362(4)	C14	C19	1.522(4)
N1	B	1.551(4)	C15	C16	1.545(5)
N2	C1	1.341(4)	C15	C17	1.533(5)

N3	N4	1.374(4)	C15	C18	1.529(5)
N3	C14	1.364(4)	C19	C20	1.542(4)
N3	B	1.572(4)	C19	C21	1.531(5)
N4	C12	1.353(4)	C19	C22	1.537(4)
N5	N6	1.387(4)	C23	C24	1.412(4)
N5	C25	1.371(4)	C23	C26	1.519(4)
N5	B	1.562(4)	C24	C25	1.384(4)
N6	C23	1.323(4)	C25	C30	1.523(4)
C1	C2	1.399(5)	C26	C27	1.539(5)
C1	C4	1.515(4)	C26	C28	1.533(5)
C2	C3	1.390(4)	C26	C29	1.541(5)
C3	C8	1.523(4)	C30	C31	1.537(5)
C4	C5	1.529(5)	C30	C32	1.538(5)
C4	C6	1.545(5)	C30	C33	1.541(5)
C4	C7	1.535(5)	C34	C35	1.410(5)
C8	C9	1.542(5)			

Table S7. Bond Angles for [HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N4	Au	N2	85.59(10)	N4	C12	C15	122.5(3)
C34	Au	N2	116.70(12)	C13	C12	C15	128.3(3)
C34	Au	N4	157.63(13)	C14	C13	C12	107.0(3)
C35	Au	N2	155.54(13)	N3	C14	C13	106.9(3)
C35	Au	N4	118.71(12)	N3	C14	C19	126.4(3)
C35	Au	C34	39.20(14)	C13	C14	C19	126.5(3)
N2	N1	B	117.7(2)	C12	C15	C16	108.9(3)
C3	N1	N2	109.9(2)	C12	C15	C17	110.6(3)
C3	N1	B	132.3(3)	C12	C15	C18	110.4(3)
N1	N2	Au	112.47(19)	C17	C15	C16	108.2(3)
C1	N2	Au	129.5(2)	C18	C15	C16	108.1(3)
C1	N2	N1	107.1(3)	C18	C15	C17	110.7(3)
N4	N3	B	117.1(2)	C14	C19	C20	108.6(3)
C14	N3	N4	110.0(2)	C14	C19	C21	112.5(3)
C14	N3	B	132.7(3)	C14	C19	C22	109.8(3)
N3	N4	Au	112.46(18)	C21	C19	C20	107.4(3)
C12	N4	Au	128.8(2)	C21	C19	C22	111.0(3)
C12	N4	N3	107.0(3)	C22	C19	C20	107.4(3)
N6	N5	B	114.8(2)	N6	C23	C24	110.5(3)
C25	N5	N6	109.7(2)	N6	C23	C26	121.2(3)
C25	N5	B	134.0(3)	C24	C23	C26	128.2(3)

C23	N6	N5	106.8(3)	C25	C24	C23	105.8(3)
N2	C1	C2	109.3(3)	N5	C25	C24	107.2(3)
N2	C1	C4	123.2(3)	N5	C25	C30	126.5(3)
C2	C1	C4	127.5(3)	C24	C25	C30	126.2(3)
C3	C2	C1	106.7(3)	C23	C26	C27	110.6(3)
N1	C3	C2	106.9(3)	C23	C26	C28	110.1(3)
N1	C3	C8	125.7(3)	C23	C26	C29	108.3(3)
C2	C3	C8	127.5(3)	C27	C26	C29	109.1(3)
C1	C4	C5	112.2(3)	C28	C26	C27	109.5(3)
C1	C4	C6	109.2(3)	C28	C26	C29	109.1(3)
C1	C4	C7	108.5(3)	C25	C30	C31	111.5(3)
C5	C4	C6	109.9(3)	C25	C30	C32	110.0(3)
C5	C4	C7	108.1(3)	C25	C30	C33	109.5(3)
C7	C4	C6	108.8(3)	C31	C30	C32	110.1(3)
C3	C8	C9	111.4(3)	C31	C30	C33	107.7(3)
C3	C8	C10	112.8(3)	C32	C30	C33	108.0(3)
C3	C8	C11	108.5(3)	C35	C34	Au	69.6(2)
C10	C8	C9	108.9(3)	C34	C35	Au	71.2(2)
C11	C8	C9	107.7(3)	N1	B	N3	106.7(2)
C11	C8	C10	107.3(3)	N1	B	N5	107.8(2)
N4	C12	C13	109.1(3)	N5	B	N3	112.6(3)

Computational Details

Calculations were done using the ADF2019 code.[16] Triple-ξ and two polarization functions (STO-TZ2P) basis sets were employed within the generalized gradient approximation (GGA) according to the BP86 exchange-correlation functional and the empirical dispersion correction to DFT (DFT-D) given by the pair-wise Grimme correction (D3)[17] and Becke-Johnson damping functions.[18] Molecular structures were optimized through the analytical energy gradient method implemented by Versluis and Ziegler[19] at the TZ2P/BP86-D3 level without any symmetry restrain, resulting in a κ^2-coordination fashion. For optimization of κ^3-coordination, the three ^{Pz}N-Au distances were set to be equal. The energy convergence criterion was set to 10^{-5} Hartree, gradient convergence criteria to 10^{-4} Hartree/Å, and radial convergence criteria to 10^{-3} Å, to achieve final relaxed structures.

A quantitative analysis of the interaction nature of the Au-ethylene bond is obtained via the interaction energy ΔE_{int} between [HB(3,5-(R)$_2$Pz)$_3$]Au and (C_2H_4) fragments. The energy decomposition analysis (EDA)[20] describes ΔE_{int} in terms of different meaningful quantities accounting for the electrostatic interaction (ΔE_{elstat}) between the defined fragments, the repulsive exchange (ΔE_{Pauli}) interaction owing to the four-electron/two-orbital repulsion between occupied orbitals from the different fragments. The orbital (covalent) interaction (ΔE_{orb}), which comes from the orbital relaxation and the orbital mixing between the fragments. Moreover, the dispersion interaction (ΔE_{disp}) was evaluated via the pairwise correction of Grimme[17d] (DFT-D3), denoting a stabilizing character. The counterpoise method was employed to overcome the basis set superposition error (BSSE), denoting values lower than 2.0 kcal mol^{-1}. According to:

$$\Delta E_{int} = \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$$

Table S8. Calculated Au-ethylene bonding energy (kcal·mol^{-1}), and energy decomposition analysis. Contribution from backdonation and donation schemes (kcal·mol^{-1}) to bonding formation, in addition, the population of π_1 and π^*_2 orbitals (a.u.) of ethylene, C=C and Au-C bond distances (Å), C=C stretch ($\nu_{C=C}$, cm^{-1}), and calculated ^{1}H and ^{13}C NMR (ppm) for coordinated ethylene, are given for the relaxed κ^2- coordination for comparison.

	κ^2-[HB(3,5-(CF$_3$)$_2$Pz)$_3$]Au(C$_2$H$_4$)		κ^2-[HB(Pz)$_3$]Au(C$_2$H$_4$)		κ^2-[HB(3,5-(Me)$_2$Pz)$_3$]Au(C$_2$H$_4$)		κ^2-[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)	
ΔE_{Pauli}	197.8		207.9		217.2		222.9	
ΔE_{Elstat}	-160.0	61.1%	-168.5	61.5%	-172.9	61.0%	-169.7	59.9%
ΔE_{Orb}	-95.2	36.3%	-102.0	37.2%	-104.5	36.9%	-103.7	36.6%
ΔE_{Disp}	-6.8	2.6%	-3.4	1.3%	-5.9	2.1%	-10.1	3.5%
ΔE_{int}	-64.3		-66.0		-66.1		-60.6	
Au←π-C$_2$H$_4$	-36.0	37.8%	-32.3	31.7%	-32.3	30.9%	-36.0	34.7%
Au→π*-C$_2$H$_4$	-46.5	48.8%	-58.2	57.0%	-60.5	57.9%	-53.3	51.4%
Ethylene								
Pop. π_1	1.47		1.56		1.54		1.45	
Pop. π^*_2	0.31		0.43		0.47		0.37	
IR $\nu_{C=C}$	1492		1481		1480		1488	
Dist. C=C	1.416		1.427		1.427		1.418	
Dist. Au-C	2.126		2.112		2.112		2.126	
^{1}H-NMR	4.1		3.3		3.3		3.4	
^{13}C-NMR	66.5		53.2		50.5		62.2	

Table S9. Calculated Au-ethylene bonding energy (kcal·mol^{-1}), and energy decomposition analysis. Contribution from backdonation and donation schemes (kcal·mol^{-1}) to bonding formation, in addition, the population of π_1 and π^*_2 orbitals (a.u.) of ethylene, C=C and Au-C bond distances (Å), C=C stretching ($\nu_{C=C}$, cm^{-1}), and calculated ^{1}H and ^{13}C NMR (ppm) for coordinated ethylene, are given for the relaxed κ^2- coordination, and restricted κ^3-fashion for comparison. Calculated values for free ethylene: IR $\nu_{C=C}$ 1635 (Exp: 1623); C=C distance 1.331 Å (Exp: 1.3305);[11] ^{1}H NMR 5.81 ppm (Exp: 5.4 ppm); ^{13}C NMR 124.11 ppm (Exp: 123.13 ppm).

	[HB(3,5-(CF$_3$)$_2$Pz)$_3$]Au(C$_2$H$_4$)				**[HB(3,5-(CH$_3$)$_2$Pz)$_3$]Au(C$_2$H$_4$)**				**[HB(3,5-(*t*-Bu)$_2$Pz)$_3$]Au(C$_2$H$_4$)**			
	κ^2–		κ^3–		κ^2–		κ^3–		κ^2–		κ^3–	
ΔE_{Pauli}	197.8		188.3		217.2		209.0		222.9		214.3	
ΔE_{Elstat}	-160.0	61.1%	-151.4	61.4%	-172.9	61.0%	-163.4	61.7%	-169.7	59.9%	-159.0	60.3%
ΔE_{Orb}	-95.2	36.3%	-88.4	35.9%	-104.5	36.9%	-95.9	36.2%	-103.7	36.6%	-94.8	35.9%
ΔE_{Disp}	-6.8	2.6%	-6.6	2.7%	-5.9	2.1%	-5.6	2.1%	-10.1	3.5%	-10.1	3.8%
ΔE_{int}	-64.3		-58.1		-66.1		-55.9		-60.6		-49.5	
Au←π-C$_2$H$_4$	-36.0	37.8%	-35.9	40.6%	-32.3	30.9%	-32.6	33.9%	-36.0	34.7%	-35.3	37.2%
Au→π*-C$_2$H$_4$	-46.5	48.8%	-39.7	44.9%	-60.5	57.9%	-50.8	52.9%	-53.3	51.4%	-44.5	47.0%
Ethylene												
Pop. π_1	1.47		1.47		1.54		1.58		1.45		1.44	
Pop. π^*_2	0.31		0.28		0.47		0.34		0.37		0.30	
IR $\nu_{C=C}$	1492		1501		1480		1493		1488		1501	
Dist. C=C	1.416		1.407		1.427		1.415		1.418		1.406	
Dist. Au-C	2.126		2.146		2.112		2.139		2.126		2.178	
^{1}H-NMR	4.1		4.4		3.3		3.9		3.4		3.9	
^{13}C-NMR	66.5		73.1		50.5		58.0		62.2		70.6	

	[HB(Pz)$_3$]Au(C$_2$H$_4$)				**[HB(3,5-(Ph)$_2$Pz)$_3$]Au(C$_2$H$_4$)**			
	κ^2–		κ^3–		κ^2–		κ^3–	
ΔE_{Pauli}	207.9		201.8		213.8		205.6	
ΔE_{Elstat}	-168.5	61.5%	-160.8	62.4%	-166.7	59.8%	-157.9	60.4%
ΔE_{Orb}	-102.0	37.2%	-93.7	36.4%	-101.1	36.3%	-92.8	35.5%
ΔE_{Disp}	-3.4	1.3%	-3.2	1.3%	-10.8	3.9%	-10.6	4.1%
ΔE_{int}	-66.0		-55.9		-64.8		-55.7	
Au←π-C$_2$H$_4$	-32.3	31.7%	-32.5	34.6%	-34.9	34.5%	-34.5	37.2%
Au→π*-C$_2$H$_4$	-58.2	57.0%	-48.9	52.2%	-51.9	51.3%	-44.0	47.4%
Ethylene								
Pop. π_1	1.56		1.57		1.36		1.39	
Pop. π^*_2	0.43		0.36		0.31		0.22	
IR $\nu_{C=C}$	1481		1493		1478		1494	
Dist. C=C	1.427		1.414		1.420		1.409	
Dist. Au-C	2.112		2.131		2.126		2.149	
^{1}H-NMR	3.3		3.7		2.4		3.0	
^{13}C-NMR	53.2		60.1		60.0		68.2	

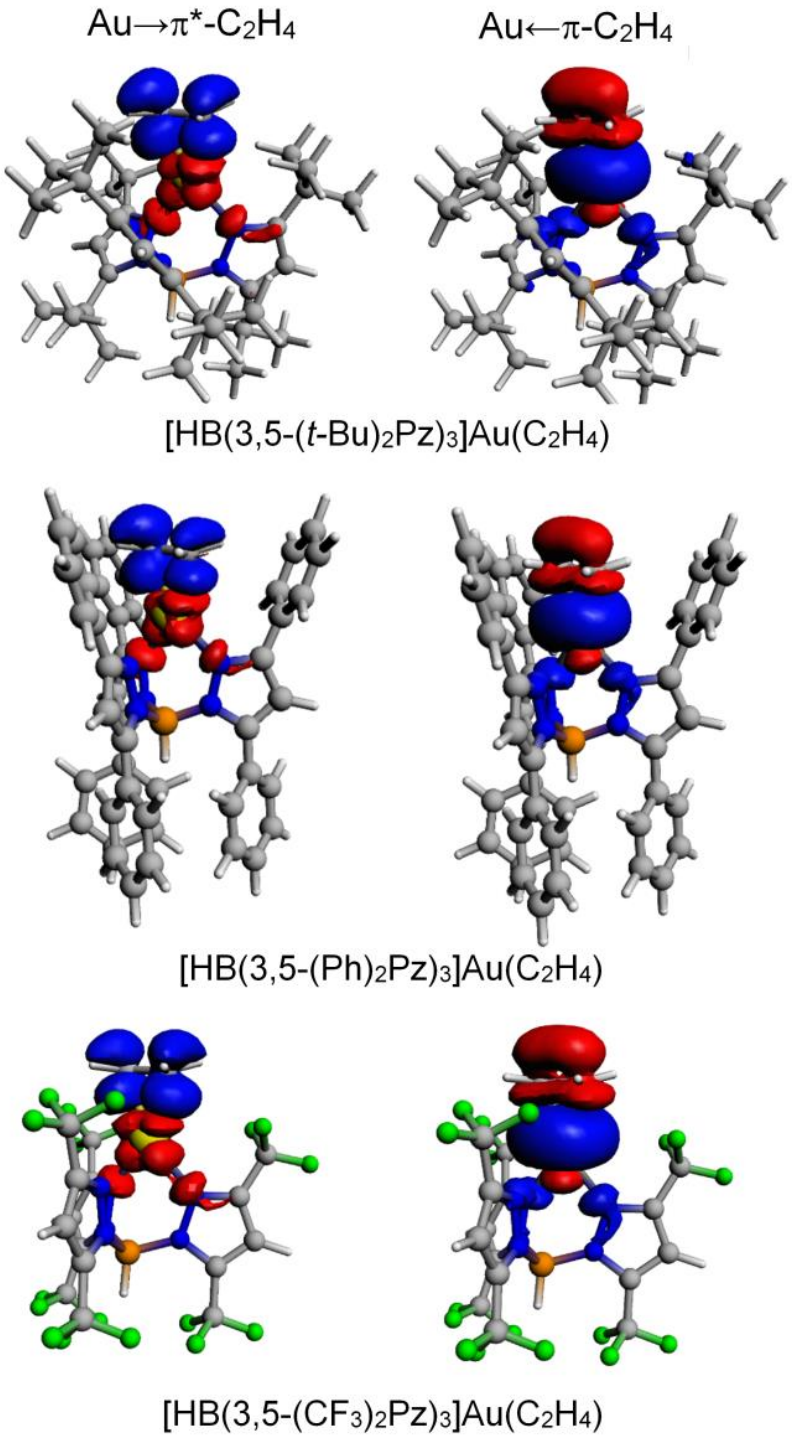

Figure S9. Deformation density contributing to ΔE_{Orb}, accounting for Au→π*-C_2H_4 backdonation (left) and Au←π-C_2H_4 σ-donation (right) bonding schemes.

Table S10. Cartesian coordinates (Å) for the optimized structures in both κ^2- and κ^3-coordination fashion, in a Multiple XYZ format.

```
106
Kappa2-[HB(3,5-(t-Bu)2Pz)3]Au(C2H4)
Au        3.730243000      3.972701000      4.256740000
N         6.445580000      4.609903000      5.579299000
N         5.122804000      4.525497000      5.938318000
N         6.234065000      2.280856000      4.655676000
N         4.984115000      2.156071000      4.105360000
N         6.710233000      4.306418000      3.092272000
N         5.923995000      5.432604000      3.110806000
C         4.929936000      5.368768000      6.971017000
C         6.137443000      6.024769000      7.250560000
H         6.306998000      6.763060000      8.021494000
C         7.078995000      5.542181000      6.340957000
C         3.595711000      5.559346000      7.666397000
C         2.726061000      4.292310000      7.578743000
H         2.478433000      4.037431000      6.540488000
H         1.785760000      4.447554000      8.125226000
H         3.247344000      3.430152000      8.014292000
C         2.867117000      6.756119000      7.015419000
H         2.733459000      6.587745000      5.941897000
H         3.451688000      7.677225000      7.140215000
H         1.880220000      6.904920000      7.476502000
C         3.839462000      5.874797000      9.156768000
H         2.877441000      5.993893000      9.673763000
H         4.403424000      6.807161000      9.288055000
H         4.397021000      5.064508000      9.644817000
C         8.513247000      6.019406000      6.151253000
C         8.757562000      6.410812000      4.676267000
H         8.751101000      5.540914000      4.012700000
H         9.736008000      6.902063000      4.584756000
H         7.979416000      7.097460000      4.321318000
C         9.546835000      4.961411000      6.593507000
H         9.386738000      4.669384000      7.639646000
H        10.560004000      5.377308000      6.502841000
H         9.495902000      4.061302000      5.973049000
C         8.726727000      7.276621000      7.019971000
H         8.022519000      8.073895000      6.748406000
H         9.745854000      7.655322000      6.867989000
H         8.609094000      7.055406000      8.089117000
C         4.605146000      0.866753000      4.225973000
C         5.618193000      0.163371000      4.888802000
H         5.617580000     -0.888824000      5.134104000
C         6.630971000      1.079334000      5.171486000
C         3.289334000      0.332845000      3.693323000
C         3.314499000     -1.206875000      3.696776000
H         4.150794000     -1.593770000      3.099386000
H         2.380382000     -1.591025000      3.265754000
H         3.401136000     -1.607513000      4.715680000
C         2.124520000      0.797674000      4.595569000
H         2.252858000      0.412428000      5.615767000
H         1.166266000      0.429752000      4.202297000
H         2.081827000      1.891711000      4.657721000
C         3.090250000      0.813777000      2.240781000
H         3.137479000      1.903736000      2.167910000
H         2.116724000      0.476446000      1.858662000
H         3.877177000      0.403361000      1.594085000
C         7.883444000      0.823047000      5.995789000
C         7.843578000     -0.621951000      6.535295000
H         6.947849000     -0.801594000      7.144073000
H         8.723155000     -0.794905000      7.169146000
H         7.867639000     -1.358441000      5.720953000
C         9.180367000      0.969454000      5.173364000
H         9.174459000      0.288688000      4.312298000
H        10.045849000      0.721387000      5.802968000
H         9.313858000      1.986613000      4.798110000
C         7.886572000      1.782693000      7.205589000
H         7.860678000      2.829973000      6.896228000
```

```
H        8.789391000      1.623094000      7.811392000
H        7.006963000      1.600786000      7.837149000
C        5.939916000      5.940315000      1.877963000
C        6.731157000      5.134858000      1.033104000
H        6.939152000      5.290394000     -0.017859000
C        7.218567000      4.102154000      1.829807000
C        5.199145000      7.221921000      1.552571000
C        3.919985000      6.889016000      0.755834000
H        4.162480000      6.329941000     -0.157781000
H        3.388721000      7.808381000      0.469117000
H        3.238823000      6.274798000      1.356874000
C        4.825475000      7.962476000      2.848562000
H        4.249737000      7.318814000      3.523392000
H        4.235598000      8.859609000      2.614434000
H        5.726401000      8.268553000      3.395877000
C        6.101567000      8.131245000      0.693444000
H        7.039583000      8.355266000      1.218397000
H        5.590248000      9.079649000      0.474682000
H        6.354223000      7.655949000     -0.263746000
C        8.171288000      2.996024000      1.412666000
C        7.618329000      1.606781000      1.787511000
H        7.570749000      1.462959000      2.868046000
H        8.265306000      0.821529000      1.371916000
H        6.604440000      1.472742000      1.388486000
C        9.552609000      3.223178000      2.064959000
H        9.977183000      4.180934000      1.736150000
H       10.246250000      2.418301000      1.782586000
H        9.480310000      3.243970000      3.156745000
C        8.356379000      3.031737000     -0.117665000
H        7.400510000      2.883991000     -0.637791000
H        9.039444000      2.227336000     -0.422421000
H        8.790585000      3.983372000     -0.450873000
C        2.078888000      5.259830000      3.822411000
H        1.347178000      5.255540000      4.631428000
H        2.434974000      6.247318000      3.526689000
C        2.109984000      4.185530000      2.897192000
H        2.501122000      4.339607000      1.890006000
H        1.399917000      3.363427000      2.991686000
B        6.971940000      3.651325000      4.480637000
H        8.140802000      3.462399000      4.643478000
105
Kappa3-[HB(3,5-(t-Bu)2Pz)3]Au(C2H4)
Au       3.638020000      3.924941000      4.286098000
N        6.362001000      4.758267000      5.677253000
N        5.095938000      4.479095000      6.116745000
N        6.375219000      2.417238000      4.694789000
N        5.218544000      2.131898000      4.019042000
N        6.506893000      4.444988000      3.169807000
N        5.341438000      5.175224000      3.136981000
C        4.863589000      5.244030000      7.197198000
C        5.991863000      6.043470000      7.442315000
H        6.116276000      6.763137000      8.239484000
C        6.924457000      5.730600000      6.453144000
C        3.552955000      5.213732000      7.956732000
C        2.940832000      3.801231000      7.924427000
H        2.774212000      3.458268000      6.897088000
H        1.979042000      3.796567000      8.455872000
H        3.611272000      3.078315000      8.406762000
C        2.587839000      6.234942000      7.314284000
H        2.456015000      6.016527000      6.250104000
H        2.989744000      7.252853000      7.401286000
H        1.605866000      6.204951000      7.807691000
C        3.793830000      5.611845000      9.425746000
H        2.849359000      5.559458000      9.984345000
H        4.173446000      6.638528000      9.511050000
H        4.515549000      4.937383000      9.904617000
C        8.272028000      6.392591000      6.208182000
C        8.336818000      6.911977000      4.755830000
H        8.262868000      6.102915000      4.023787000
H        9.287758000      7.437422000      4.591126000
H        7.513234000      7.611014000      4.562283000
```

C	9.454465000	5.441869000	6.492150000
H	9.419828000	5.075648000	7.526461000
H	10.403097000	5.978001000	6.348245000
H	9.450653000	4.575065000	5.825329000
C	8.411377000	7.602211000	7.153931000
H	7.597823000	8.323927000	7.003186000
H	9.361778000	8.113671000	6.954026000
H	8.412819000	7.293388000	8.207855000
C	4.994756000	0.811816000	4.146780000
C	6.011201000	0.245334000	4.931622000
H	6.113607000	-0.794693000	5.208542000
C	6.869305000	1.286498000	5.282132000
C	3.793436000	0.127776000	3.526549000
C	4.069930000	-1.379244000	3.368515000
H	4.963129000	-1.554706000	2.754665000
H	3.213922000	-1.865058000	2.879072000
H	4.218504000	-1.867641000	4.340615000
C	2.576460000	0.308684000	4.461301000
H	2.757217000	-0.189663000	5.423348000
H	1.670604000	-0.123886000	4.012046000
H	2.400041000	1.370385000	4.673068000
C	3.512852000	0.722725000	2.133186000
H	3.403604000	1.810544000	2.172709000
H	2.595636000	0.287063000	1.711462000
H	4.344597000	0.504249000	1.450637000
C	8.070583000	1.216074000	6.212349000
C	8.153025000	-0.197994000	6.821823000
H	7.240239000	-0.447149000	7.379270000
H	9.000294000	-0.244591000	7.519017000
H	8.309954000	-0.962615000	6.049147000
C	9.398030000	1.481876000	5.470948000
H	9.551179000	0.741819000	4.674801000
H	10.237035000	1.410014000	6.176475000
H	9.421221000	2.477158000	5.016298000
C	7.883528000	2.221634000	7.368967000
H	7.844638000	3.252962000	7.012154000
H	8.716352000	2.135088000	8.080467000
H	6.945101000	2.021090000	7.902053000
C	5.261049000	5.720016000	1.910004000
C	6.353313000	5.294988000	1.133063000
H	6.562786000	5.557925000	0.104901000
C	7.127544000	4.478678000	1.952683000
C	4.184285000	6.703927000	1.494561000
C	3.272165000	6.051674000	0.434243000
H	3.850840000	5.755836000	-0.450557000
H	2.485233000	6.750248000	0.115298000
H	2.794297000	5.148356000	0.831891000
C	3.350137000	7.177970000	2.693853000
H	2.820026000	6.349383000	3.171439000
H	2.608818000	7.917690000	2.362095000
H	3.988666000	7.636407000	3.459147000
C	4.868730000	7.941019000	0.868120000
H	5.551056000	8.410915000	1.588764000
H	4.112882000	8.682171000	0.572640000
H	5.448108000	7.672887000	-0.023955000
C	8.397027000	3.729247000	1.581064000
C	8.268739000	2.237300000	1.952716000
H	8.187972000	2.086564000	3.030951000
H	9.154698000	1.690650000	1.598535000
H	7.375784000	1.797960000	1.488814000
C	9.634722000	4.353226000	2.261473000
H	9.780964000	5.385787000	1.918656000
H	10.535332000	3.776336000	2.007779000
H	9.539507000	4.374486000	3.351539000
C	8.605252000	3.817850000	0.055547000
H	7.752811000	3.391443000	-0.488920000
H	9.506177000	3.254714000	-0.223156000
H	8.746527000	4.855285000	-0.274896000
C	1.508788000	4.351137000	4.450316000
H	1.097824000	3.791219000	5.290635000
H	1.336559000	5.426680000	4.478308000

```
C        1.782607000      3.707456000      3.230323000
H        1.818878000      4.284779000      2.306530000
H        1.553656000      2.649705000      3.105527000
B        6.933112000      3.863775000      4.541647000
H        8.124613000      3.839479000      4.618462000
93
Kappa2-[HB(3,5-(Ph)2Pz)3]Au(C2H4)
Au       1.307100000      4.433900000      3.286500000
N        3.686100000      2.659500000      2.200500000
N        2.406100000      3.051300000      1.936800000
N        4.446100000      4.561800000      3.668000000
N        3.288800000      5.273900000      3.723500000
N        3.769200000      2.331000000      4.727800000
N        2.450100000      2.516700000      4.979300000
B        4.423800000      3.015900000      3.515600000
C        2.062800000      2.536000000      0.739200000
C        3.137300000      1.791900000      0.226400000
H        3.173700000      1.250300000     -0.710400000
C        4.151200000      1.888500000      1.175300000
C        5.488100000      1.267800000      1.165500000
C        5.599100000     -0.127400000      1.079300000
H        4.692400000     -0.727900000      1.019900000
C        6.852700000     -0.740300000      1.100300000
H        6.923700000     -1.824400000      1.044200000
C        8.008700000      0.034800000      1.204200000
H        8.987100000     -0.443400000      1.229700000
C        7.906600000      1.426000000      1.276400000
H        8.799000000      2.043600000      1.360500000
C        6.656800000      2.038700000      1.252500000
H        6.585000000      3.122400000      1.315500000
C        3.604200000      6.582400000      3.741500000
C        4.996900000      6.721400000      3.678700000
H        5.571300000      7.639800000      3.688100000
C        5.505900000      5.422400000      3.626500000
C        6.911900000      5.011100000      3.487300000
C        7.515400000      4.105600000      4.370600000
H        6.939000000      3.692000000      5.193900000
C        8.847000000      3.731900000      4.198500000
H        9.291600000      3.020900000      4.892000000
C        9.594800000      4.256400000      3.142800000
H       10.633900000      3.955800000      3.006100000
C        9.007600000      5.172100000      2.266800000
H        9.584100000      5.590300000      1.444700000
C        7.675300000      5.548600000      2.438500000
H        7.206400000      6.248600000      1.747600000
C        2.216600000      2.046400000      6.216300000
C        3.417500000      1.559200000      6.783400000
H        3.557900000      1.062000000      7.736200000
C        4.389000000      1.741000000      5.806900000
C        5.800100000      1.338800000      5.855400000
C        6.569600000      1.634000000      6.994700000
H        6.113500000      2.195600000      7.809500000
C        7.904400000      1.238700000      7.075000000
H        8.487200000      1.484100000      7.961700000
C        8.492000000      0.538500000      6.018500000
H        9.535900000      0.232600000      6.076900000
C        7.733300000      0.233400000      4.885400000
H        8.176200000     -0.312600000      4.054500000
C        6.400300000      0.626400000      4.803900000
H        5.814600000      0.374500000      3.921300000
C       -0.287700000      5.421800000      4.270100000
H       -0.287000000      5.131800000      5.322600000
H       -0.247400000      6.493800000      4.075400000
C       -0.824900000      4.535000000      3.300400000
H       -1.183200000      4.911900000      2.342200000
H       -1.274700000      3.593800000      3.614700000
H        5.549600000      2.653300000      3.428500000
C        0.741200000      2.771700000      0.138900000
C        0.634800000      3.286500000     -1.160800000
C       -0.428900000      2.478500000      0.852600000
C       -0.617800000      3.522400000     -1.727100000
```

```
C       -1.680700000      2.719400000      0.289000000
C       -1.779400000      3.245600000     -1.000900000
H        1.544100000      3.516800000     -1.716000000
H       -0.342000000      2.058300000      1.852200000
H       -0.688000000      3.930600000     -2.734100000
H       -2.582400000      2.493400000      0.857400000
H       -2.757700000      3.436700000     -1.440400000
C        2.536500000      7.601200000      3.803900000
C        1.802000000      7.916700000      2.652400000
C        2.199100000      8.207800000      5.020600000
C        0.741400000      8.820500000      2.716600000
C        1.136400000      9.110500000      5.086400000
C        0.403900000      9.416300000      3.935200000
H        2.058900000      7.430000000      1.712700000
H        2.760400000      7.946900000      5.918100000
H        0.172500000      9.053300000      1.817000000
H        0.873000000      9.567700000      6.040100000
H       -0.429900000     10.116100000      3.988000000
C        0.862000000      2.063200000      6.776800000
C       -0.251700000      2.206900000      5.931400000
C        0.638100000      1.940000000      8.158400000
C       -1.542700000      2.260700000      6.450200000
C       -0.657000000      1.975600000      8.676900000
C       -1.753900000      2.145400000      7.827800000
H       -0.076100000      2.268300000      4.859800000
H        1.488700000      1.829100000      8.831100000
H       -2.392700000      2.382900000      5.777700000
H       -0.812000000      1.878800000      9.751100000
H       -2.763700000      2.182000000      8.235500000
93
Kappa3-[HB(3,5-(Ph)2Pz)3]Au(C2H4)
Au       1.257052000      4.230681000      3.559830000
N        3.761257000      2.694978000      2.132222000
N        2.522586000      3.159923000      1.815124000
N        4.523726000      4.591957000      3.636598000
N        3.391802000      5.291771000      3.890465000
N        3.750143000      2.399520000      4.640225000
N        2.398571000      2.460740000      4.724989000
B        4.477658000      3.060253000      3.449693000
C        2.180512000      2.616604000      0.632528000
C        3.218632000      1.778133000      0.182845000
H        3.241682000      1.188222000     -0.724711000
C        4.203186000      1.839609000      1.163072000
C        5.460410000      1.074270000      1.277236000
C        5.393470000     -0.324976000      1.358403000
H        4.418438000     -0.809840000      1.311224000
C        6.552982000     -1.083615000      1.531495000
H        6.482597000     -2.168079000      1.604511000
C        7.794575000     -0.451236000      1.623096000
H        8.700520000     -1.041114000      1.765216000
C        7.870881000      0.940061000      1.528503000
H        8.831910000      1.446496000      1.602163000
C        6.714407000      1.699604000      1.352771000
H        6.781827000      2.785401000      1.294592000
C        3.730388000      6.588424000      3.992630000
C        5.116866000      6.727250000      3.790430000
H        5.698102000      7.641053000      3.800945000
C        5.592377000      5.440215000      3.556981000
C        6.954098000      5.006978000      3.194101000
C        7.692424000      4.123115000      3.994081000
H        7.264489000      3.751051000      4.924440000
C        8.962702000      3.709406000      3.596522000
H        9.513828000      3.012409000      4.225819000
C        9.515247000      4.173428000      2.400458000
H       10.505892000      3.841694000      2.088646000
C        8.792373000      5.064234000      1.603880000
H        9.213606000      5.429643000      0.668016000
C        7.521081000      5.480162000      2.000556000
H        6.942966000      6.160340000      1.375836000
C        2.055532000      1.995972000      5.942186000
C        3.216177000      1.656005000      6.665486000
```

```
H        3.280268000      1.198342000      7.645104000
C        4.279576000      1.908207000      5.801834000
C        5.717140000      1.679480000      6.009388000
C        6.346319000      2.195344000      7.153050000
H        5.756730000      2.771174000      7.865778000
C        7.713481000      2.004335000      7.360404000
H        8.189963000      2.424685000      8.245802000
C        8.469182000      1.289707000      6.428608000
H        9.537720000      1.144958000      6.586744000
C        7.848057000      0.761579000      5.293716000
H        8.425151000      0.205644000      4.556810000
C        6.483246000      0.949135000      5.085668000
H        6.007516000      0.533577000      4.197921000
C       -0.347239000      5.061765000      4.696233000
H       -0.446339000      4.482321000      5.617276000
H       -0.169579000      6.131242000      4.818656000
C       -0.882069000      4.554902000      3.495233000
H       -1.117595000      5.216012000      2.660620000
H       -1.405823000      3.598488000      3.500750000
H        5.593569000      2.663376000      3.400839000
C        0.891068000      2.892400000     -0.015495000
C        0.843092000      3.257506000     -1.369767000
C       -0.311450000      2.774935000      0.696194000
C       -0.378568000      3.515112000     -1.991596000
C       -1.532328000      3.040470000      0.078238000
C       -1.570712000      3.411799000     -1.268910000
H        1.775884000      3.356256000     -1.924494000
H       -0.274049000      2.460052000      1.736442000
H       -0.399754000      3.807993000     -3.041085000
H       -2.457863000      2.948089000      0.646418000
H       -2.524289000      3.617072000     -1.754438000
C        2.727005000      7.623645000      4.283048000
C        1.567813000      7.741584000      3.499809000
C        2.911249000      8.504162000      5.359077000
C        0.602331000      8.700377000      3.805314000
C        1.945441000      9.463620000      5.663812000
C        0.785040000      9.560881000      4.891961000
H        1.432584000      7.072147000      2.650740000
H        3.809301000      8.412806000      5.969870000
H       -0.291525000      8.780092000      3.189682000
H        2.096447000     10.131840000      6.511897000
H        0.030182000     10.308867000      5.132878000
C        0.641973000      1.868498000      6.307184000
C       -0.319522000      1.585808000      5.320305000
C        0.214599000      2.034315000      7.633475000
C       -1.670878000      1.499540000      5.647041000
C       -1.138658000      1.937772000      7.961081000
C       -2.088171000      1.677476000      6.969420000
H        0.015336000      1.434077000      4.295519000
H        0.950574000      2.261131000      8.404883000
H       -2.403055000      1.278814000      4.869726000
H       -1.454363000      2.074947000      8.994524000
H       -3.145178000      1.604685000      7.225855000
51
Kappa2-[HB(3,5-(CF3)2Pz)3]Au(C2H4)
Au       3.222802000      3.547681000      3.695918000
N        3.972284000      6.616586000      3.296645000
N        4.470801000      5.355687000      3.254726000
N        1.818605000      6.278778000      4.585437000
N        2.074371000      5.000786000      4.959408000
N        1.773521000      6.272179000      2.030427000
N        1.731979000      4.929717000      1.912741000
B        2.431346000      6.899287000      3.285613000
C        5.807542000      5.459431000      3.249948000
C        6.203040000      6.796939000      3.295517000
H        7.206268000      7.199183000      3.307665000
C        5.010013000      7.499643000      3.329635000
C        6.682125000      4.243756000      3.217472000
C        4.863016000      8.987323000      3.464028000
C        1.440168000      4.794249000      6.122559000
C        0.752231000      5.941288000      6.523786000
```

```
H        0.150441000      6.087824000      7.409888000
C        1.018413000      6.860525000      5.522893000
C        1.493818000      3.466541000      6.816084000
C        0.491682000      8.263176000      5.440191000
C        1.155713000      4.664978000      0.739778000
C        0.799427000      5.842796000      0.065429000
H        0.312648000      5.954103000     -0.894090000
C        1.209317000      6.850191000      0.922069000
C        1.018269000      3.244931000      0.292357000
C        1.110669000      8.323373000      0.677341000
C        3.803438000      1.657372000      2.918018000
C        2.689586000      1.491172000      3.775652000
F        6.430462000      3.463098000      2.134773000
F        6.510627000      3.464239000      4.320100000
F        7.986692000      4.608172000      3.172241000
F        4.213158000      9.554005000      2.423354000
F        4.194468000      9.321159000      4.597634000
F        6.096170000      9.552727000      3.534733000
F        2.766294000      3.012915000      6.958337000
F        0.803760000      2.511201000      6.135066000
F        0.945072000      3.561843000      8.051636000
F       -0.297886000      8.509631000      6.518151000
F       -0.260157000      8.452049000      4.328417000
F        1.473724000      9.195049000      5.434888000
F        2.227346000      2.703942000     -0.045924000
F        0.498480000      2.446634000      1.264321000
F        0.216495000      3.150787000     -0.796676000
F        0.400991000      8.553101000     -0.458404000
F        0.494642000      8.987501000      1.684670000
F        2.335795000      8.890732000      0.510398000
H        2.258809000      8.075984000      3.290531000
H        3.663890000      1.660971000      1.836425000
H        4.807562000      1.406879000      3.261821000
H        2.825675000      1.114076000      4.789303000
H        1.690533000      1.364278000      3.357062000
51
Kappa3-[HB(3,5-(CF3)2Pz)3]Au(C2H4)
Au      -0.251310000     -0.011779000      1.998051000
N        1.465047000      0.123250000     -0.834772000
N        1.619979000     -0.103543000      0.489816000
N       -0.815088000      1.215179000     -1.020003000
N       -0.887391000      1.552628000      0.285727000
N       -0.606954000     -1.322864000     -1.025525000
N       -0.986562000     -1.501051000      0.258630000
B        0.059234000      0.009365000     -1.485830000
C        2.921706000      0.064637000      0.754056000
C        3.636544000      0.411938000     -0.398648000
H        4.694400000      0.610001000     -0.503622000
C        2.670533000      0.440589000     -1.390352000
C        3.433939000     -0.079216000      2.151502000
C        2.860533000      0.816455000     -2.827819000
C       -1.681305000      2.625814000      0.371672000
C       -2.144683000      3.008351000     -0.891519000
H       -2.795340000      3.832466000     -1.148375000
C       -1.571250000      2.084624000     -1.750170000
C       -1.992115000      3.236515000      1.702570000
C       -1.763619000      1.993534000     -3.234813000
C       -1.523259000     -2.723052000      0.344821000
C       -1.496297000     -3.369938000     -0.895535000
H       -1.850911000     -4.360228000     -1.145344000
C       -0.903833000     -2.446306000     -1.740751000
C       -2.010295000     -3.252308000      1.657999000
C       -0.564569000     -2.638238000     -3.189079000
F        2.937881000     -1.184045000      2.770232000
F        3.092459000      0.990648000      2.930198000
F        4.785720000     -0.166893000      2.161920000
F        2.491798000     -0.164226000     -3.686639000
F        2.143774000      1.927318000     -3.148282000
F        4.169727000      1.092485000     -3.059913000
F       -0.867328000      3.500274000      2.418406000
F       -2.763370000      2.415863000      2.471204000
```

```
F       -2.669227000      4.399518000      1.543920000
F       -2.635577000      2.953284000     -3.639067000
F       -2.279708000      0.791351000     -3.598761000
F       -0.613345000      2.169558000     -3.927331000
F       -0.976637000     -3.547097000      2.497386000
F       -2.804048000     -2.362235000      2.310139000
F       -2.722269000     -4.390647000      1.475707000
F       -0.920420000     -3.890555000     -3.576199000
F       -1.202087000     -1.764183000     -4.003481000
F        0.769696000     -2.503074000     -3.409617000
H        0.152145000      0.021989000     -2.671734000
C       -0.184464000     -0.744072000      4.012695000
C       -0.120889000      0.661785000      4.031255000
H       -1.122224000     -1.259091000      4.221554000
H        0.722369000     -1.337232000      4.136645000
H        0.835922000      1.165909000      4.170435000
H       -1.008858000      1.253548000      4.254584000
72
Kappa2-[HB(3-(CF3)5-(Ph)Pz)3]Au(C2H4)
Au       1.239286000      4.398605000      3.207523000
N        3.689851000      2.692739000      2.206921000
N        2.376491000      2.947063000      1.976619000
N        4.360717000      4.652490000      3.656377000
N        3.210663000      5.365614000      3.556798000
N        3.708565000      2.447724000      4.765993000
N        2.456743000      2.804548000      5.135438000
B        4.373988000      3.103391000      3.541166000
C        2.063390000      2.347747000      0.816246000
C        3.174935000      1.693937000      0.281936000
H        3.239704000      1.154337000     -0.653911000
C        4.209504000      1.943980000      1.184291000
C        0.690751000      2.448090000      0.234216000
C        5.618045000      1.541582000      1.068744000
C        5.932191000      0.223436000      0.702505000
H        5.125716000     -0.492126000      0.543510000
C        7.262195000     -0.174729000      0.568493000
H        7.492330000     -1.202057000      0.289353000
C        8.294046000      0.736794000      0.805258000
H        9.332910000      0.421424000      0.715002000
C        7.989272000      2.053489000      1.157826000
H        8.783245000      2.775297000      1.344189000
C        6.661917000      2.457191000      1.276880000
H        6.432551000      3.490502000      1.528012000
C        3.555046000      6.662372000      3.600647000
C        4.939948000      6.803257000      3.716223000
H        5.509096000      7.719339000      3.800645000
C        5.431985000      5.498964000      3.754907000
C        2.521664000      7.740702000      3.577506000
C        6.828568000      5.053782000      3.865211000
C        7.217835000      4.080405000      4.797140000
H        6.480248000      3.661028000      5.478054000
C        8.540467000      3.648064000      4.855332000
H        8.815585000      2.874880000      5.570554000
C        9.496622000      4.196267000      3.997067000
H       10.529923000      3.853273000      4.041347000
C        9.124788000      5.186618000      3.084315000
H        9.866219000      5.622062000      2.415194000
C        7.797748000      5.612191000      3.016659000
H        7.498208000      6.365327000      2.288023000
C        2.226446000      2.187442000      6.296136000
C        3.334898000      1.429011000      6.710017000
H        3.430583000      0.797321000      7.584564000
C        4.275648000      1.606404000      5.700793000
C        0.929864000      2.368869000      7.009981000
C        5.615798000      1.013874000      5.599429000
C        6.464382000      1.025642000      6.719085000
H        6.121603000      1.497154000      7.639819000
C        7.738325000      0.462574000      6.649582000
H        8.385881000      0.482772000      7.525532000
C        8.186894000     -0.112327000      5.457538000
H        9.186721000     -0.541208000      5.398644000
```

```
C        7.345410000     -0.139145000      4.343094000
H        7.678566000     -0.587735000      3.408741000
C        6.067033000      0.408940000      4.416420000
H        5.408161000      0.360732000      3.552336000
C       -0.472993000      5.344243000      4.030721000
H       -0.426552000      5.287019000      5.119390000
H       -0.585799000      6.347960000      3.619043000
C       -0.874174000      4.209938000      3.276689000
H       -1.297946000      4.333863000      2.278952000
H       -1.137736000      3.280918000      3.784661000
F        0.325936000      3.735411000     -0.023560000
F       -0.264506000      1.931596000      1.056265000
F        0.622682000      1.767033000     -0.940665000
F        1.710659000      7.704473000      4.672222000
F        1.705246000      7.666949000      2.489574000
F        3.114759000      8.963889000      3.557914000
F       -0.054267000      2.835366000      6.197370000
F        1.030315000      3.252050000      8.050510000
F        0.491282000      1.195129000      7.551800000
H        5.502241000      2.748212000      3.492358000
72
Kappa3-[HB(3-(CF3)5-(Ph)Pz)3]Au(C2H4)
Au       1.179600000      4.294100000      3.590200000
N        3.764100000      2.817500000      2.145200000
N        2.488500000      3.190400000      1.897800000
N        4.466000000      4.616600000      3.810400000
N        3.323100000      5.322000000      3.970700000
N        3.665000000      2.363400000      4.643900000
N        2.358000000      2.631300000      4.872100000
B        4.428400000      3.096400000      3.518200000
C        2.165000000      2.697400000      0.697200000
C        3.236000000      1.982100000      0.148800000
H        3.289900000      1.499000000     -0.818000000
C        4.252900000      2.080400000      1.097300000
C        0.812000000      2.941100000      0.117300000
C        5.609500000      1.516000000      1.031000000
C        5.769800000      0.155900000      0.721900000
H        4.885600000     -0.458500000      0.555100000
C        7.043300000     -0.408500000      0.651600000
H        7.152700000     -1.466700000      0.418800000
C        8.171900000      0.380500000      0.884000000
H        9.167100000     -0.060600000      0.831900000
C        8.021000000      1.737600000      1.177200000
H        8.891900000      2.365300000      1.356900000
C        6.750100000      2.303900000      1.247000000
H        6.642300000      3.363700000      1.469900000
C        3.680600000      6.603300000      4.117200000
C        5.071700000      6.746200000      4.046600000
H        5.656900000      7.649400000      4.160700000
C        5.552100000      5.451900000      3.854900000
C        2.648800000      7.654400000      4.351200000
C        6.950100000      5.012200000      3.722400000
C        7.481800000      3.991300000      4.524600000
H        6.855000000      3.506700000      5.270900000
C        8.808700000      3.594000000      4.372500000
H        9.197100000      2.791800000      4.997500000
C        9.625900000      4.217700000      3.426700000
H       10.663200000      3.905200000      3.308800000
C        9.110000000      5.245300000      2.633800000
H        9.740400000      5.736400000      1.893900000
C        7.780500000      5.641400000      2.781300000
H        7.368300000      6.431500000      2.154300000
C        2.021900000      1.943100000      5.969900000
C        3.116300000      1.230700000      6.478700000
H        3.144000000      0.565600000      7.332200000
C        4.160400000      1.515000000      5.601200000
C        0.626900000      2.005000000      6.494100000
C        5.549100000      1.031700000      5.640100000
C        6.293200000      1.160700000      6.823700000
H        5.829900000      1.625000000      7.693900000
C        7.618000000      0.725600000      6.877800000
```

```
H        8.186300000      0.838600000      7.800300000
C        8.214700000      0.156800000      5.750100000
H        9.251600000     -0.176500000      5.790000000
C        7.476600000      0.013000000      4.572700000
H        7.928300000     -0.429000000      3.686000000
C        6.151400000      0.439400000      4.519600000
H        5.579100000      0.313600000      3.602500000
C       -0.554000000      5.257800000      4.384200000
H       -0.706300000      4.918000000      5.409800000
H       -0.443200000      6.335300000      4.253400000
C       -0.938100000      4.440500000      3.301000000
H       -1.127700000      4.875200000      2.318500000
H       -1.389800000      3.463600000      3.481600000
F        0.478800000      4.261600000      0.104500000
F       -0.176300000      2.303100000      0.809500000
F        0.752600000      2.494000000     -1.165800000
F        1.904000000      7.413000000      5.467300000
F        1.763700000      7.763100000      3.318300000
F        3.233000000      8.872600000      4.508000000
F       -0.307500000      1.740700000      5.537200000
F        0.311300000      3.236800000      6.999900000
F        0.444800000      1.108000000      7.499000000
H        5.540800000      2.693400000      3.480300000
33
Kappa2-[HB(3,5-(H)2Pz)3]Au(C2H4)
Au       3.350705000      3.554010000      3.883619000
N        4.025181000      6.561333000      3.337307000
N        4.570151000      5.323994000      3.488880000
N        1.850695000      6.206889000      4.596278000
N        2.008570000      4.904272000      4.955544000
N        1.851682000      6.240707000      2.051138000
N        1.917966000      4.914038000      1.753681000
B        2.492176000      6.821020000      3.319709000
C        5.901750000      5.457770000      3.380839000
C        6.233298000      6.799294000      3.151185000
H        7.219185000      7.227245000      3.020736000
C        5.012619000      7.462752000      3.130266000
C        1.258434000      4.697314000      6.049144000
C        0.597196000      5.878619000      6.409253000
H       -0.076944000      6.035373000      7.241694000
C        1.001053000      6.809225000      5.459940000
C        1.260456000      4.767639000      0.598414000
C        0.758606000      6.000612000      0.132517000
H        0.190119000      6.197142000     -0.768694000
C        1.159815000      6.915909000      1.092885000
C        4.086883000      1.691032000      3.203933000
C        2.857932000      1.500500000      3.902761000
H        2.312429000      8.013709000      3.346660000
H        4.104724000      1.660643000      2.112639000
H        5.030743000      1.430047000      3.685556000
H        2.868202000      1.093182000      4.915617000
H        1.936147000      1.322552000      3.346226000
H        0.744897000      7.854140000      5.332308000
H        1.241206000      3.717021000      6.511551000
H        1.009055000      7.986825000      1.168315000
H        1.174311000      3.783118000      0.148321000
H        4.772527000      8.508536000      2.980831000
H        6.539234000      4.586124000      3.475593000
33
Kappa3-[HB(3,5-(H)2Pz)3]Au(C2H4)
Au      -0.204915000     -0.001007000      2.048943000
N        1.422732000      0.068745000     -0.818372000
N        1.652706000      0.058364000      0.522310000
N       -0.825532000      1.231282000     -0.933624000
N       -1.049145000      1.507839000      0.377286000
N       -0.706563000     -1.306309000     -0.925740000
N       -0.909635000     -1.590120000      0.386958000
B       -0.007643000     -0.004186000     -1.393012000
C        2.979712000      0.153682000      0.680208000
C        3.626275000      0.227955000     -0.565718000
H        4.687881000      0.308891000     -0.764446000
```

```
C        2.595191000      0.170721000     -1.493696000
C       -1.771941000      2.634571000      0.425725000
C       -2.024981000      3.105716000     -0.872450000
H       -2.576718000      3.990742000     -1.163980000
C       -1.406045000      2.182188000     -1.705506000
C       -1.542815000     -2.769074000      0.441263000
C       -1.758530000     -3.266214000     -0.854229000
H       -2.241517000     -4.192273000     -1.139729000
C       -1.211331000     -2.303431000     -1.692281000
H        0.046799000     -0.003773000     -2.597330000
C        0.097094000     -0.710130000      4.035326000
C       -0.034489000      0.697587000      4.059450000
H       -0.740014000     -1.343916000      4.335569000
H        1.083591000     -1.170054000      4.118059000
H        0.852460000      1.326085000      4.161692000
H       -0.970818000      1.155377000      4.381630000
H        2.607000000      0.193284000     -2.577159000
H        3.403338000      0.162645000      1.679440000
H       -1.329402000      2.131887000     -2.784847000
H       -2.065343000      3.046962000      1.384862000
H       -1.140094000     -2.251351000     -2.772019000
H       -1.809131000     -3.195681000      1.402189000
51
Kappa2-[HB(3,5-(CH3)2Pz)3]Au(C2H4)
Au       3.274414000      3.583171000      3.852027000
N        4.038270000      6.578871000      3.390105000
N        4.551382000      5.320130000      3.539051000
N        1.845493000      6.248588000      4.642417000
N        2.025252000      4.943747000      5.008680000
N        1.865525000      6.283671000      2.097467000
N        1.897933000      4.940451000      1.860078000
B        2.507475000      6.855157000      3.373443000
C        5.887539000      5.400187000      3.432265000
C        6.247225000      6.737053000      3.205430000
H        7.246922000      7.135342000      3.077193000
C        5.054663000      7.456314000      3.180621000
C        6.745306000      4.183064000      3.536709000
C        4.844203000      8.918143000      2.961833000
C        1.266062000      4.707116000      6.090122000
C        0.576451000      5.881164000      6.429106000
H       -0.114298000      6.022840000      7.251984000
C        0.961538000      6.836399000      5.491866000
C        1.235913000      3.359285000      6.731172000
C        0.522747000      8.257542000      5.362985000
C        1.290390000      4.741532000      0.687571000
C        0.852019000      5.974122000      0.151238000
H        0.325747000      6.146665000     -0.781466000
C        1.234889000      6.937622000      1.075882000
C        1.158283000      3.359296000      0.131639000
C        1.034974000      8.417749000      1.043268000
C        3.907678000      1.739182000      3.040260000
C        2.686892000      1.557004000      3.757027000
H        6.641458000      3.552847000      2.641707000
H        6.451536000      3.572388000      4.400744000
H        7.799646000      4.461154000      3.643190000
H        4.230592000      9.106194000      2.070509000
H        4.333863000      9.385017000      3.814152000
H        5.812271000      9.411447000      2.823050000
H        2.254493000      2.989321000      6.909270000
H        0.731455000      2.628411000      6.082307000
H        0.703202000      3.396894000      7.687640000
H       -0.182597000      8.498211000      6.166133000
H        0.025423000      8.437304000      4.400577000
H        1.371355000      8.951420000      5.425561000
H        1.692393000      3.256818000     -0.823823000
H        1.578619000      2.634579000      0.839936000
H        0.106653000      3.096028000     -0.049382000
H        0.495122000      8.698794000      0.131793000
H        0.453952000      8.769820000      1.907141000
H        1.991060000      8.959648000      1.055066000
H        2.344060000      8.044114000      3.398770000
```

```
H        3.897266000      1.781597000      1.950039000
H        4.849065000      1.399818000      3.475626000
H        2.698540000      1.077527000      4.737012000
H        1.745819000      1.459709000      3.212998000
51
Kappa3-[HB(3,5-(CH3)2Pz)3]Au(C2H4)
Au       3.047422000      3.502256000      3.487976000
N        4.004975000      6.631217000      3.339096000
N        4.517598000      5.367722000      3.378134000
N        1.815389000      6.322297000      4.597517000
N        1.921781000      5.007596000      4.944050000
N        1.857942000      6.211709000      2.058257000
N        1.908874000      4.855735000      1.898478000
B        2.474375000      6.876948000      3.307689000
C        5.853035000      5.466647000      3.401838000
C        6.215774000      6.826354000      3.375616000
H        7.216696000      7.242359000      3.387543000
C        5.020522000      7.537670000      3.337003000
C        6.715741000      4.248773000      3.436299000
C        4.799611000      9.014408000      3.304834000
C        1.259123000      4.827626000      6.093318000
C        0.710248000      6.056764000      6.504965000
H        0.122431000      6.251767000      7.394619000
C        1.080910000      6.982509000      5.535007000
C        1.171288000      3.479987000      6.728676000
C        0.778386000      8.442967000      5.458986000
C        1.318459000      4.575178000      0.728724000
C        0.876010000      5.766287000      0.121121000
H        0.357302000      5.875016000     -0.824851000
C        1.235543000      6.788866000      0.992910000
C        1.221648000      3.166706000      0.237202000
C        1.017365000      8.261496000      0.868899000
C        3.731568000      1.615380000      2.774559000
C        2.631534000      1.409469000      3.639966000
H        7.069697000      3.981267000      2.429889000
H        6.147521000      3.398120000      3.833101000
H        7.597153000      4.409145000      4.069509000
H        4.249619000      9.321419000      2.405051000
H        4.219253000      9.354854000      4.173005000
H        5.765494000      9.531813000      3.311584000
H        1.966240000      2.830639000      6.341161000
H        0.205438000      3.000441000      6.513025000
H        1.272738000      3.550294000      7.819241000
H        0.163839000      8.737073000      6.317172000
H        0.232145000      8.694721000      4.539977000
H        1.695862000      9.047133000      5.468050000
H        2.073881000      2.908733000     -0.408998000
H        1.216737000      2.467483000      1.082438000
H        0.304456000      3.014535000     -0.345109000
H        0.496807000      8.480410000     -0.070171000
H        0.411977000      8.652457000      1.698089000
H        1.967689000      8.812716000      0.872165000
H        2.277812000      8.060014000      3.258278000
H        3.594989000      1.565645000      1.693000000
H        4.745617000      1.412570000      3.121713000
H        2.797276000      1.052366000      4.657202000
H        1.642344000      1.194910000      3.232187000
```

References:

1. H. V. R. Dias and J. Wu, *Organometallics*, 2012, **31**, 1511-1517.
2. H. V. R. Dias and J. Wu, *Angew. Chem., Int. Ed.*, 2007, **46**, 7814-7816.
3. S. G. Ridlen, J. Wu, N. V. Kulkarni and H. V. R. Dias, *Eur. J. Inorg. Chem.*, 2016, 2573-2580.
4. Y. Yang, P. Antoni, M. Zimmer, K. Sekine, F. F. Mulks, L. Hu, L. Zhang, M. Rudolph, F. Rominger and A. S. K. Hashmi, *Angew. Chem., Int. Ed.*, 2019, **58**, 5129-5133.
5. M. J. Harper, C. J. Arthur, J. Crosby, E. J. Emmett, R. L. Falconer, A. J. Fensham-Smith, P. J. Gates, T. Leman, J. E. McGrady, J. F. Bower and C. A. Russell, *J. Am. Chem. Soc.*, 2018, **140**, 4440-4445.
6. J. A. Flores and H. V. R. Dias, *Inorg. Chem.*, 2008, **47**, 4448-4450.
7. K. Klimovica, K. Kirschbaum and O. Daugulis, *Organometallics*, 2016, **35**, 2938-2943.
8. J. Schaefer, D. Himmel and I. Krossing, *Eur. J. Inorg. Chem.*, 2013, **2013**, 2712-2717.
9. H. V. R. Dias, M. Fianchini, T. R. Cundari and C. F. Campana, *Angew. Chem., Int. Ed.*, 2008, **47**, 556-559.
10. G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176-2179.
11. N. C. Craig, P. Groner and D. C. McKean, *J. Phys. Chem. A*, 2006, **110**, 7461-7469.
12. C. M. Dowling, D. Leslie, M. H. Chisholm and G. Parkin, *Main Group Chem.*, 1995, **1**, 29-52.
13. N. Kitajima, K. Fujisawa, C. Fujimoto and Y. Moro-oka, *Chem. Lett.*, 1989, **18**, 421-424.
14. M. Sheldrick George, *Acta Crystallogr A*, 2008, **64**, 112-122.
15. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.
16. (a) G. te Velde and E. J. Baerends, *Phys. Rev. B.*, 1991, **44**, 7888-7903; (b) C. Fonseca Guerra, J. G. Snijders, G. te Velde and E. J. Baerends, *Theor. Chem. Accounts Theory, Comput. Model. (Theoretica Chim. Acta)*, 1998, **99**, 391-403.
17. (a) S. Grimme, *J. Comput. Chem.*, 2004, **25**, 1463-1473; (b) S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787-1799; (c) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104; (d) S. Grimme, *Rev. Comput. Mol. Sci.*, 2011, **1**, 211-228.
18. (a) E. R. Johnson and A. D. Becke, *J. Chem. Phys.*, 2005, **123**, 024101; (b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465.
19. L. Versluis and T. Ziegler, *J. Chem. Phys.*, 1988, **88**, 322-328.
20. (a) K. Morokuma, *J. Chem. Phys.*, 1971, **55**, 1236-1244; (b) T. Ziegler and A. Rauk, *Theoret. Chim. Acta*, 1977, **46**, 1-10; (c) M. v. Hopffgarten and G. Frenking, *Rev. Comput. Mol. Sci.*, 2012, **2**, 43-62.