Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Relationship between the anion/cation relative orientation and the catalytic activity for nitrogen acyclic carbene-gold catalysts

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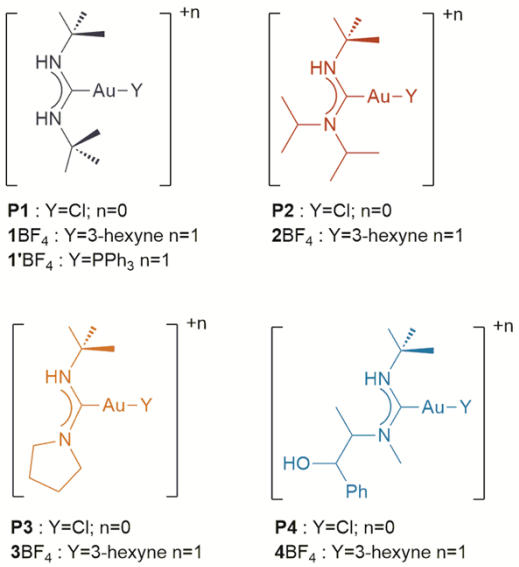
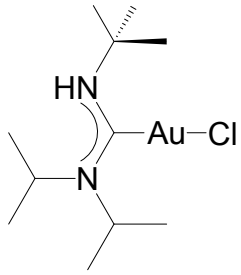
1. General procedures

$HAuCl_4$, tetrahydrothiophene (THT), *tert*-Butylisocianide, *tert*-Buthylamine, diisopropylamine, pyrrolidine, (1R,2S)-(−)-Ephedrine, $AgBF_4$, AgOTf, N,N'-dicyclohexylurea (DCU), triphenylphosphine and 3-hexyne were purchased from Ricci Chimica and Sigma Aldrich. AgBF4 was charged in Schlenk flask and stored under nitrogen atmosphere at -20°C. (THT)AuCl,[1] [t*ert*-Butylisocianide]-gold(I) Chloride, **P1** and **P3** were synthesized according to the literature methods or with minor modifications. All manipulations of moisture-sensitive materials were performed using flamed Schlenk glassware on a Schlenk line, interfaced to a high vacuum pump. Pentane and CH_2Cl_2 were distilled after 12 hours of reflux over Na and CaH_2, respectively, and freeze-pump-thaw degassed. CD_2Cl_2 and $CDCl_3$ was freeze-pump-thaw degassed over CaH_2 and vacuum transferred into storage Schlenk flasks. All the new compound were characterized in solution by ^1H, ^{13}C, ^{19}F, NMR spectroscopies. One- and two dimensional ^1H, ^{13}C, and ^{19}F NMR spectra were measured on Bruker DRX 400 spectrometers. Referencing is relative to TMS (^1H and ^{13}C) and CCl_3F(^{19}F). The elemental analyses were carried out with a Carlo Erba 1106 elemental analyzer.

2. Synthesis and characterization.



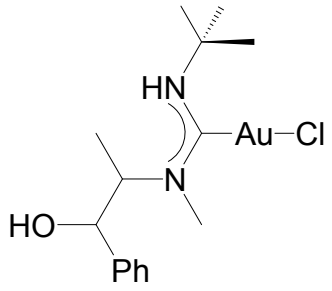
Scheme S1. Structure of **P1-P4**, **1-4**BF_4 and **1'**BF_4 complexes.



[(*tert*-Butylamino)(di-*iso*-propyl-amino)methylidene]-gold(I) Chloride (P2).

Two equivalents of diisopropylamine were added to a solution of [*tert*-Butylisocyano]-gold(I) Chloride 221 mg (0.7 mmol) in 3 mL of acetonitrile.[2] The mixture was stirred at 60°C overnight. Then the mixture was purified by washing with Et_2O and the supernatant was removed by decantation. The crude product was washed with pentane and then all volatiles was removed under vacuum. The product was recrystallized from dichloromethane/pentane. We obtained the product as a white-yellow solid; yield: 245 mg (91.3%). Anal. Calcd. for $C_{11}H_{24}AuClN_2$ (416.74): C, 31.70; H, 5.80; Au, 47.26; Cl, 8.51; N, 6.72. Found: C, 31.65; H, 5.84; N, 6.62.

^{1}H NMR (400.13 MHz, CD_2Cl_2, 297K): δ = 6.20 (br s, 1H, N*H*), 5.36 (m, 1H, C*H*Me$_2$), 3.86 (m, 1H, C*H*Me$_2$), 1.63 (s, 9H, ^{t}Bu), 1.40 (d, *J* = 6.9 Hz, 6H, CH*Me*), 1.25 (d, J = 5.5 Hz, 6H, CH*Me*). **^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, 297K):** δ = 190.45 (s, $C_{carbene}$), 54.46 (s, *C*Me$_3$), 45.38 (s, *C*HMe$_2$), 31.73 (s, C*Me*$_3$), 29.88 (s, *C*HMe$_2$), 21.00 (s, CH*Me*$_2$), 20.72 (s, CH*Me*$_2$).

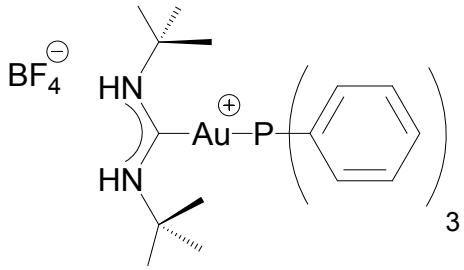


[((1R,2S)-1-phenyl-1-propanol-2-amino)(*tert*-Butylamino)methylidene]-gold(I) Chloride (P4).

Two equivalents of (1R,2S)-(−)-Ephedrine were added to a solution of [*tert*-Butylisocyano]-gold(I) Chloride complex 56.8 mg (0.18 mmol) in 2 mL of CH_2Cl_2. The mixture was stirred at room temperature and protected from the light for 3 days. The mixture was concentrated and precipitate with pentane. We obtained the product as a white solid; yield: 80 mg (92.3%). Anal. Calcd. for $C_{15}H_{24}AuClN_2O$ (480.78): C, 37.47; H, 5.03; Au, 40.97; Cl, 7.37; N, 5.83; O, 3.33. Found: C, 37.53; H, 5.12; N, 5.69.

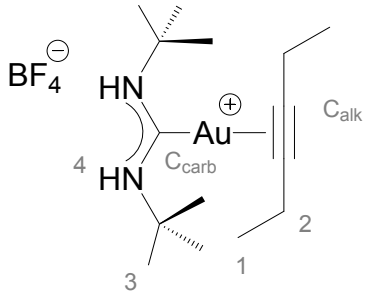
^{1}H NMR (400.13 MHz, CD_2Cl_2, 297 K): δ =7.53 (d, 2H, J_3^{HH} = 7.4 Hz, *o*-Ph), 7.41 (t, 2H, J_3^{HH} = 7.4 Hz, *m*-Ph), 7.33 (t, 1H, J_3^{HH} = 7.4 Hz, *p*-Ph), 5.83 (br s, 1H, N*H*), 5.38 (m, 1H, C*H*Me), 5.05 (t, 1H, J_3^{HH} = 4.0 Hz, C*H*OH), 2.88 (s, 3H, N*Me*), 2.21 (d, 1H, J_3^{HH} = 3.6 Hz, O*H*), 1.61 (s, 9H, C*Me*$_3$), 1.31 (d, 3H, J_3^{HH} = 6.9 Hz, CH*Me*) ppm. **^{13}C{^{1}H} NMR (100.5 MHz, CD_2Cl_2, 297 K):** δ = 191.15 (s,

$C_{carbene}$), 140.96 (s, C_{ipso}), 128.60 (s, C_{Ph}), 128.08 (s, $C_{p\text{-}Ph}$), 125.93 (s, C_{Ph}), 70.34 (s, *C*OH), 59.46 (s, *C*Me), 54.29 (s, *C*Me_3), 38.10 (s, N*Me*), 30.85 (s, C*Me*$_3$), 12.12 (s, C*Me*) ppm.

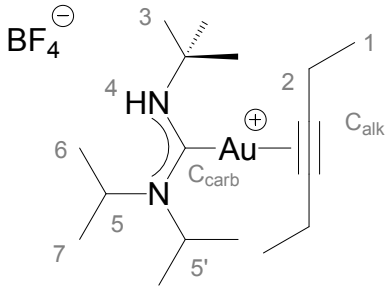


[(Bis(tert-butylamino)methylidene)](Triphenylphosphine)gold(I) tetrafluoroborate (1'BF_4).
P1 46.6 mg (0.12 mmol) and PPh_3 34.62 mg (0.13 mmol) were added in a Schlenk in 2 mL of dichloromethane, then 26 mg of $AgBF_4$ (0.13 mmol) were added. The reaction proceeds at room temperature with the concomitant precipitation of AgCl. After 30 min the reaction mixture was filtered through Celite and the solvent evaporated under reduced pressure. Then pentane was added to the crude product, which was filtered off and washed with other pentane (3x1 mL). The resulting solid was dried under vacuum. We obtained the product as a white solid; yield: 84 mg (99.9%). Anal. Calcd. for $C_{27}H_{35}AuBF_4N_2P$ (702.33): C, 46.17; H, 5.02; Au, 28.04; B, 1.54; F, 10.82; N, 3.99; P, 4.41. Found: C, 46.16; H, 5.05; N, 3.98.
^{1}H NMR (400.13 MHz, CD_3OD, 297 K): δ= 7.6 (m, 15H, PPh_3), 1.58 (s, 18H, Bu^t). **^{19}F NMR (376.42 MHz, CD_3OD, 297 K):** δ= -154.78 (br, $^{11}BF_4$), -154.83 (br, $^{10}BF_4$). **^{31}P{^{1}H} NMR (161.97 MHz, CD_3OD, 298K):** δ = 39.06. **^{13}C{^{1}H} NMR (100.5 MHz, CD_3OD, 298K):** δ = 205.1 (d, $^2J_{CP}$ = 108.9 Hz, C_{carb}), 134.0, 133.6 (d, $^2J_{CP}$ = 11.1 Hz), 132.2, 129.6, 129.5, 52.3 (s, $\underline{C}(CH_3)_3$), 30.6 (s, $C(\underline{C}H_3)_3$).

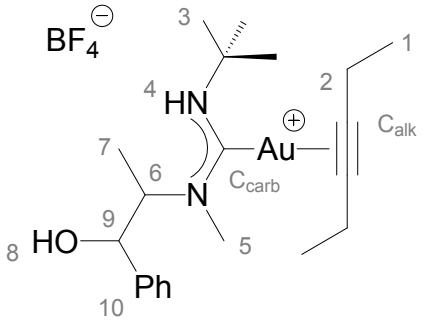
Synthetic procedure for the *in-situ* generation of 1-3BF_4 ion pairs: 1.2 equivalents of $AgBF_4$ were loaded into a screw-cap NMR tube under nitrogen atmosphere. A solution containing 1 equivalent of a Gold(I) Chloride precursor (**P1-P4**) and 1.1 equivalents of 3-hexyne dissolved in 0.6 mL of dry CD_2Cl_2 was added. The resulting mixture was strongly shaken and after some minutes a white-grey solid (AgCl and the excess of $AgBF_4$) deposited at the bottom of the tube.



1BF_4. ^{1}H NMR (400.13 MHz, CD_2Cl_2, 297 K): δ= 7.58 (br s, 2H, H4), 2.77 (br quartet, 4H, J_3^{HH} = 7.4 Hz, H2), 1.54 (s, 18H, H3), 1.34 (br t, 6H, J_3^{HH} = 7.4 Hz, H1). ^{19}F NMR (376.42 MHz, CD_2Cl_2, 297 K): δ= -149.59 (br, $^{11}BF_4$), -149.54 (br, $^{10}BF_4$). $^{13}C\{^{1}H\}$ NMR (100.5 MHz, CD_2Cl_2, 297 K): δ= 192.90 (s, C_{carb}), 87.68 (s, C_{alk}), 53.23 (s, C5), 31.66 (s, C3), 16.36 (s, C2), 14.46 (s, C1).



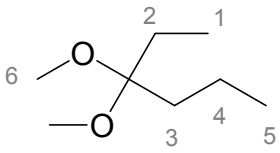
2BF_4. ^{1}H NMR (400.13 MHz, CD_2Cl_2, 297 K): δ= 6.53 (br s, 1H, H4), 4.84 (br, 1H, H5), 4.00 (br quintet, 1H, J_3^{HH} = 7.5 Hz, H5'), 2.79 (br quartet, 4H, J_3^{HH} = 7.7 Hz, H2), 1.66 (s, 9H, H3), 1.48 (br d, 6H, J_3^{HH} = 7.1 Hz, H6/H7), 1.41 (br d, 6H, J_3^{HH} = 6.6 Hz, H6/H7), 1.36 (br t, 6H, J_3^{HH} = 7.7 Hz, H1). ^{19}F NMR (376.42 MHz, CD_2Cl_2, 297 K): δ= -153.26 (br, $^{11}BF_4$), -153.20 (br, $^{10}BF_4$). $^{13}C\{^{1}H\}$ NMR (100.5 MHz, CD_2Cl_2, 297 K): δ= 192.68 (s, C_{carb}), 88.14 (s, C_{alk}), 48.96 (s), 47.17 (s), 31.83 (s), 21.15 (s), 20.71 (s), 18.88 (s), 16.02 (s, C2), 14.30 (s, C1).



4BF_4. ^{1}H NMR (400.13 MHz, CD_2Cl_2, 297 K): δ= 7.45 (m, 5H, H10), 6.29 (br s, 1H, H4), 4.90 (d, 1H, J_3^{HH} = 7.7 Hz, H9), 4.79 (quintet, 1H, J_3^{HH} = 7.5 Hz, H6), 3.86 (br, 1H, H8), 2.95 (s, 3H, H5), 2.74 (br quartet, J_3^{HH} = 7.4 Hz, H2), 1.56 (d, 3H, J_3^{HH} = 6.6 Hz, H7), 1.46 (s, 9H, H3), 1.33 (br t, J_3^{HH} = 7.1 Hz, H1). ^{19}F NMR (376.42 MHz, CD_2Cl_2, 297 K): δ= -152.22 (br, $^{11}BF_4$), -152.17 (br, $^{10}BF_4$). $^{13}C\{^{1}H\}$ NMR (100.5 MHz, CD_2Cl_2, 297 K): δ= 194.07 (s, C_{carb}), 142.91 (s, Ph_{ipso}), 128.55 (s, Ph), 128.05 (s, *p*-Ph), 125.78 (s, Ph), 87.90 (s, C_{alk}), 75.93 (s, C9), 73.12 (s, C6), 54.56 (s, *C*Me_3), 31.83 (s), 31.71 (s, C3), 30.71 (s), 16.00 (s, C2), 14.97 (s, C7), 14.36 (s, C1).

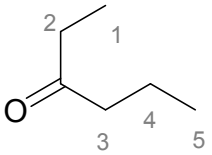
3. Alkoxylation procedure

All experiments were followed by *in situ* ^{1}H NMR. 3-hexyne (100 µL, 0.88 mmol), CH_3OH (143 µL, 3.52 mmol), TMS (5 µL) and $CDCl_3$ (400 µL) were added by syringe in a NMR tube. For the tries performed in methanol 543 µL of CD_3OD were used instead CH_3OH and chloroform-d. The content of the latter was transferred into the vial with the catalyst loading (1 mol%) and the corresponding silver activator ($AgBF_4$ or AgOTf), it was briefly shaken for a moment and quickly relocated again into NMR tube and the time count was started. The reaction mixture was further monitored by NMR at 30 °C. Conversion was calculated from the integral intensities of the corresponding signals (conversion[%] = (n_{acetal} + n_{ketone}) / ($n_{3\text{-hexyne}}$) x 100).



3,3-dimethoxyhexane - ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ (ppm) 3.15 (s, 6H, H6), 1.54 (m, 4H, H2 and H3), 1.25 (m, 2H, H4), 0.92 (t, J_3^{HH} = 7.3 Hz, 3H, H1), 0.82 (t, J_3^{HH} = 7.4 Hz, 3H, H5).

3,3-dimethoxyhexane D2 - ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ (ppm) 3.15 (s, 6H, H6), 1.59 (q, J_3^{HH} = 7.6 Hz, 2H, H2), 1.33 – 1.15 (m, 2H, H4), 0.93 (t, J_3^{HH} = 7.3 Hz, 3H, H1), 0.82 (t, J_3^{HH} = 7.5 Hz, 3H, H5).



3-hexanone - ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ (ppm) 2.36 – 2.39 (t - q, J_3^{HH} = 7.4 Hz, J_3^{HH} = 7.3 Hz, 4H, H2 and H3), 1.58 (m, 2H, H4), 1.03 (t, J_3^{HH} = 7.4 Hz, 3H, H1), 0.89 (t, J_3^{HH} = 7.4 Hz, 3H, H5).

3-hexanone D2 - ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K): δ (ppm) 2.37 (q, J_3^{HH} = 7.5 Hz, 2H, H2), 1.61-1.57 (m, 2H, H4), 1.04 (t, J_3^{HH} = 7.4 Hz, 3H, H1), 0.87 (t, J_3^{HH} = 7.3 Hz, 3H, H5).

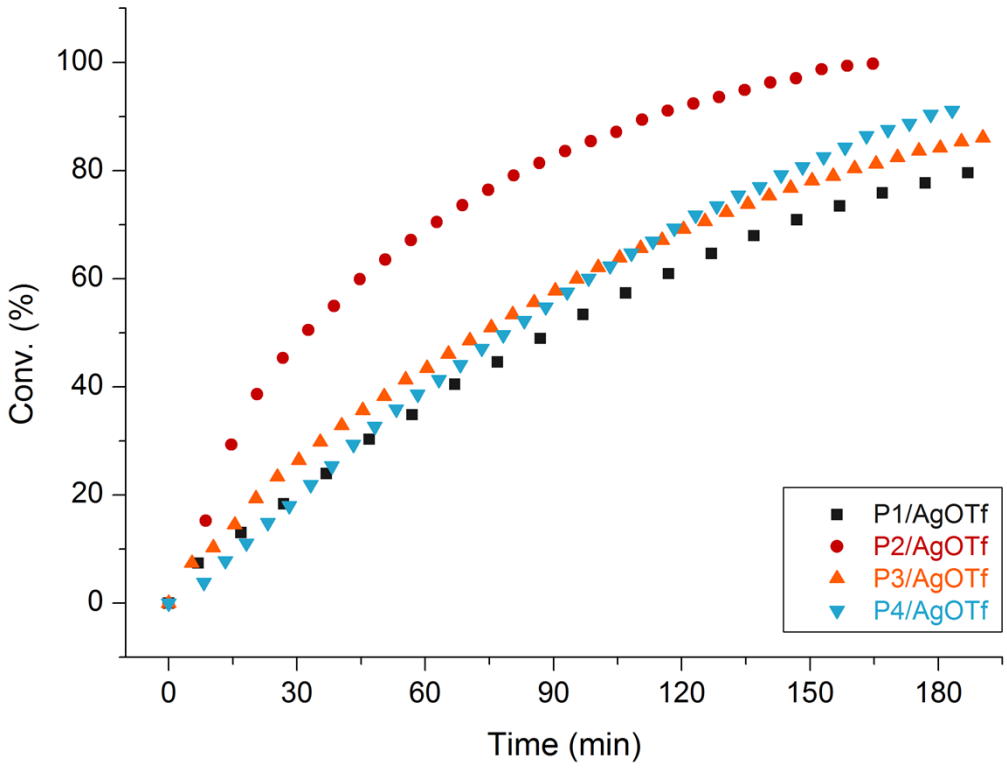


Figure S1. Alkoxylation of 3-hexyne with methanol catalyzed by **P1-P4** complexes activated with AgOTf in $CDCl_3$.

4. NOE NMR experiments

The 1H-NOESY[3] NMR experiments were acquired by the standard three-pulse sequence or by the PFG version.[4] Two-dimensional ^{19}F, ^{1}H-HOESY NMR experiments were acquired using the standard four-pulse sequence or the modified version.[5] The number of transients and the number of data points was chosen according to the sample concentration and to the desired final digital resolution. Semi-quantitative spectra were acquired using a 1s relaxation delay and 800 ms mixing times.

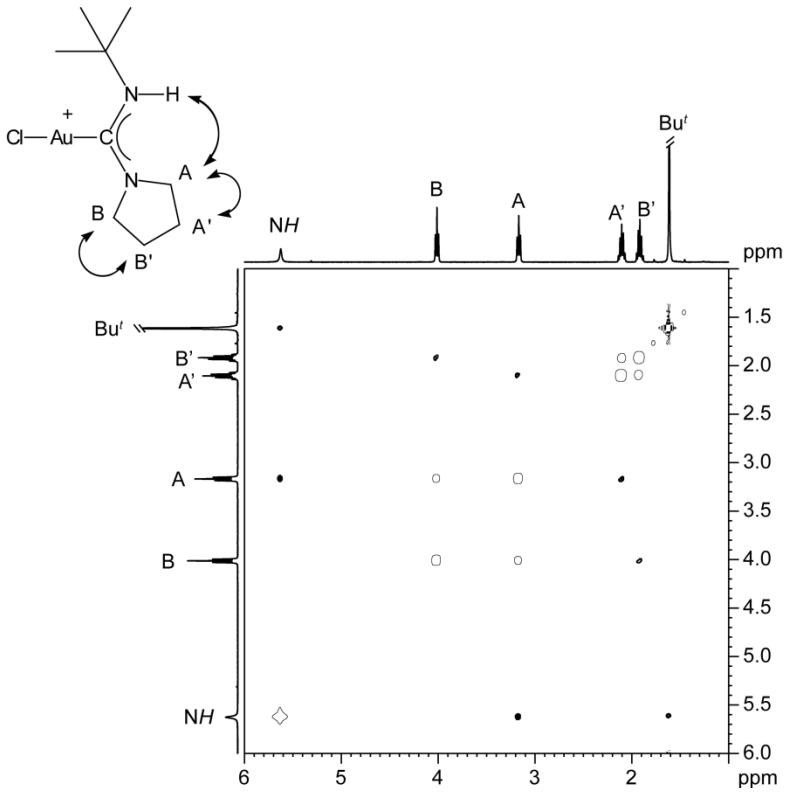


Figure S2. ^{1}H-NOESY NMR spectrum of complex **P3** (400.13 MHz, $CDCl_3$, T = 298 K). The singlet relative to the Bu^t group has a NOE contact only with the NH. The absence of NOE with protons A, A', B and B' demonstrate that the NH(Bu^t) group does not rotate around the N-C bond. The broad signal due to NH interacts only with protons A, confirming the structure depicted in the upper-left corner.

Interionic NOE NMR Studies of 1'BF_4 in CD_3OD.

Complexes **1-4**BF_4 are not stable in methanol since they react with the solvent, undergoing the nucleophilic attack of the methanol itself on the 3-hexyne. For this reason, we synthesized **1'**BF_4, in which the 3-hexyne has been substituted with the triphenylphosphine. The NH moiety is not visible in the spectrum, probably because a H/D exchange with the solvent occurs. Remarkably, the two *tert*-butyl groups are magnetically equivalent (*syn-syn* isomer).

The relative anion/cation orientation in solution of **1'**BF_4 complex has been investigated by ^{19}F, ^{1}H-HOESY NMR spectroscopy (Figure S3) in methanol-d_4 at room temperature.

A weak NOE contact is visible between BF_4^- and the two *tert*-butyl groups of the carbene (Figure S3). A very small contact is visible at 4.70 ppm, but it does not correspond with any signal. The contact could be due to the NH moiety, which is almost completely deuterated by H/D exchange with the solvent, but the remaining traces of NH are expected to give an intense NOE contact (Figure S3).

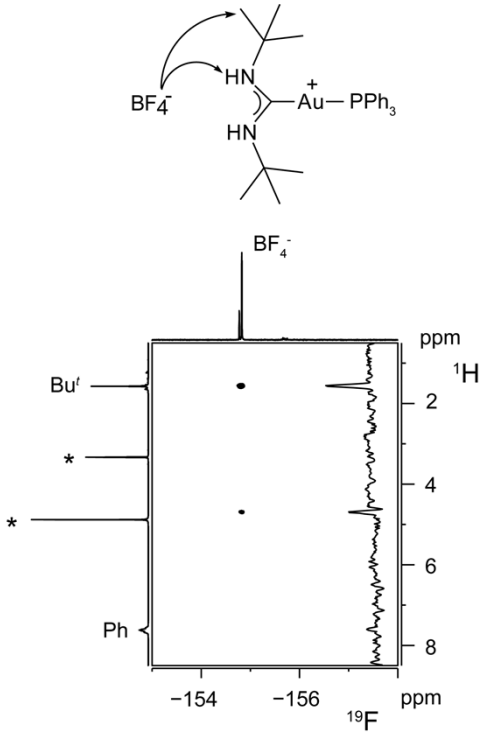


Figure S3. $^{19}F,^{1}H$-HOESY NMR spectrum (376.65 MHz, 298 K, CD_3OD) of complexes **1'**BF_4.

5. Computational details and Theoretical Method.

Equilibrium geometries and electron densities were calculated by using density functional theory (DFT) with Becke's exchange functional[6] in combination with the Lee–Yang–Parr correlation functional[7] (BLYP), using the ADF (Amsterdam Density Functional) package.[8] An all-electron triple-zeta basis set with two polarization functions was used on all atoms (TZ2P).[9] Relativistic effects were included by means of the zeroth-order regular approximation (ZORA) Hamiltonian[10,11,12] with a small frozen core. The satisfactory accuracy of this approach was verified by both coupled-cluster and all-electron four-component Dirac–Kohn–Sham calculations on closely related systems.[13] For the calculation of the ion pair structures we included the conductor like screening model (COSMO, with ε= 8.93).

The charge displacements occurring upon the formation of the bond were analyzed through the Charge Displacement Function (CDF)[14, 15, 16], defined in the following equation:

$$\Delta q = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{z} dz' \Delta\rho(x, y, z')$$

where $\Delta\rho$ is the difference between the electron density of the complex and the ones of its constituting fragments placed in the same position they occupy in the complex. In the present case, the fragments are the gold-ligand moiety and the hexyne. The CDF defines, at each point z along a chosen axis, the amount of electron charge that moves across a plane perpendicular to the z axis upon the formation of the bond. A positive (negative) value corresponds to electrons flowing in the direction of decreasing (increasing) z. Charge accumulates (decreases) where the slope is positive (negative), the difference between the Δq values computed at two points gives the amount of the charge that has flowed into (away from) the region of space delimited by the two corresponding planes.

6. DFT studies

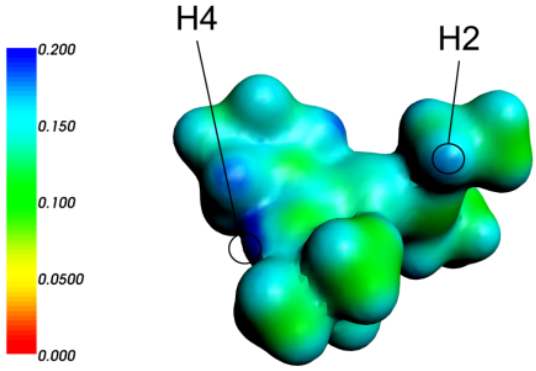
The systems **1-4**BF_4 will be thoroughly characterized by means of DFT calculations. The optimized structures, of all systems (including different ion-pair configuration) presented in the work, have been reported in the following section as Cartesian coordinates.

The interaction energies and the selected geometrical parameters for the cations **1**$^+$-**4**$^+$, in which the gold fragment is coordinated to 3-hexyne and to the corresponding NAC ligand are given in Table S1. All the systems show very similar interaction energies, around 40 kcal/mol with variations of only 2.8 kcal/mol. Also the most important geometrical parameters are very similar in all the systems. The N-Ĉ-N angles are between 116° and 119°, and the small variation well

correlate with the steric hindrance of the substituents on the nitrogen. In fact, the N-Ĉ-N angle increases according to the series **1**$^{+}$ < **4**$^{+}$= **3**$^{+}$ < **2**$^{+}$. Also the hexyne bending (180° - C-Ĉ≡C) is an important parameter. In fact, we previously shown that, in the case of acetylene, the bending occurring upon coordination to a metallic fragment is strongly related with the DCD bonding components and, in particular, with the amount of back-donation to its π* orbitals.[13] Our systems present very similar values for the hexyne bending, around 13°.

Table S1. Interaction energies (E_{int}) and most important geometrical parameters for the systems studied in this work. In the case when the system shows slight asymmetries, we reported the average of the values.

Complex	**E_{int}** (kcal/mol)	**C-N** (Å)	**N-Ĉ-N** (°)	**C-Ĉ≡C** (°)
1^{+}	-43.6	1.341	115.9	13.1
2^{+}	-40.8	1.349	118.9	13.0
3^{+}	-41.0	1.347	117.6	13.0
4^{+}	-42.1	1.341	117.6	13.0



3^{+}

Figure S4. Color-coded representation of the Coulomb potential on an electronic isodensity surface (ρ=0.007 e/A^{3}) of the cationic complex **3**$^{+}$. The regions corresponding to relevant part of the molecule are evidenced.

7. Optimized Structure in Cartesian Coordinates

1^+

C	0.598139	2.263982	-3.870643
C	0.545410	2.001224	-2.344562
C	0.215543	0.593632	-2.032307
C	-0.064201	-0.613408	-2.041718
C	-0.388199	-2.017131	-2.376406
C	-0.404103	-2.262904	-3.906195
Au	0.041162	-0.017948	0.165105
C	0.005109	-0.024036	2.236194
N	-1.140556	-0.090062	2.929576
N	1.125214	0.039524	2.970342
C	-2.576381	-0.153692	2.466576
C	2.576863	0.103335	2.559650
H	1.004290	0.037448	3.984431
H	-1.055898	-0.091973	3.947532
H	0.344721	-2.679979	-1.900331
H	-1.365316	-2.272892	-1.948497
H	1.511281	2.254085	-1.890101
H	-0.200145	2.657417	-1.879179
H	-0.647529	-3.313832	-4.094213
H	0.574190	-2.047826	-4.348949
H	-1.157650	-1.637693	-4.396652
H	-0.368612	2.052156	-4.339480
H	1.364560	1.645507	-4.349603
H	0.844216	3.317354	-4.040849
C	3.364103	0.158170	3.887998
C	2.974896	-1.165792	1.773207
C	2.852627	1.384812	1.741994
C	-3.411289	-0.213205	3.765234
C	-2.946757	1.117607	1.670215
C	-2.821229	-1.432676	1.635392
H	-3.880815	-1.494896	1.360285
H	-2.231027	-1.427686	0.711422
H	-2.557012	-2.327389	2.211390
H	-4.008719	1.084158	1.398953
H	-2.768926	2.017198	2.271428
H	-2.362889	1.195737	0.745729
H	-4.476503	-0.262990	3.517086
H	-3.155531	-1.101768	4.356207
H	-3.244726	0.680406	4.379904
H	4.045949	-1.132167	1.540472
H	2.775104	-2.067085	2.364913
H	2.424618	-1.240886	0.828100
H	4.437701	0.207581	3.678856
H	3.087803	1.045273	4.471880
H	3.174230	-0.736857	4.493776
H	3.921427	1.446955	1.505017
H	2.295896	1.383351	0.797468
H	2.568651	2.277881	2.311100

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C	0.484477	2.256166	-3.886850
C	0.440868	2.027025	-2.354923
C	0.174251	0.613526	-2.011677
Au	0.055737	0.008435	0.196121
C	-0.007353	-0.057938	2.278448
N	1.105271	-0.055758	3.043904
C	2.502808	-0.088430	2.454978
C	2.862361	1.222065	1.727986
C	-0.060120	-0.602943	-2.006600
C	-0.335851	-2.021510	-2.321743
C	-0.367743	-2.287613	-3.847852
N	-1.207614	-0.133961	2.883912
C	-2.613541	-0.095462	2.322862
C	-2.883291	-1.348897	1.460752
C	-3.531736	-0.118671	3.566107
C	-2.863545	1.206241	1.530551
H	3.148448	-0.148292	3.329606
C	2.796219	-1.352792	1.622696
C	1.009605	-0.125118	4.558232
H	-1.217725	-0.223833	3.894845
H	0.428569	-2.651071	-1.850106
H	-1.295588	-2.309601	-1.875051
H	1.392931	2.334188	-1.905073
H	-0.334899	2.659126	-1.905400
H	-0.575415	-3.349171	-4.018533
H	0.594452	-2.042694	-4.309902
H	-1.151806	-1.697181	-4.333703
H	-0.470573	1.988662	-4.351472
H	1.279058	1.661864	-4.350422
H	0.682374	3.315200	-4.083117
H	-3.920870	-1.337623	1.106317
H	-2.224422	-1.377899	0.585031
H	-2.724254	-2.263127	2.044922
H	-3.908718	1.235711	1.199941
H	-2.670841	2.085360	2.156896
H	-2.225829	1.266124	0.641006
H	-4.580300	-0.107924	3.251414
H	-3.366930	-1.025662	4.162065
H	-3.357291	0.759897	4.199967
H	3.865969	-1.374148	1.380346
H	2.553794	-2.261519	2.184846
H	2.237876	-1.367743	0.679456
H	3.922703	1.202723	1.448576
H	2.273600	1.351980	0.811482
H	2.690535	2.090420	2.373581
C	2.119180	0.650004	5.295640
H	0.086971	0.400032	4.823882
C	0.919293	-1.591417	5.033032
H	0.748385	-1.621250	6.115813
H	0.101245	-2.131444	4.542569
H	1.854596	-2.123210	4.820713
H	1.812620	0.750741	6.343270
H	3.081382	0.126756	5.288346
H	2.254710	1.656861	4.886974

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Au	0.196514	0.054848	2.333547
C	0.019646	-0.010118	4.401300
N	0.651210	-0.921310	5.159961
H	0.491935	-0.882192	6.163942
N	-0.765148	0.879077	5.023287
C	1.609309	-2.026397	4.766309
C	0.906798	-3.041141	3.837754
H	0.606129	-2.572119	2.893091
H	0.014316	-3.459795	4.317614
H	1.592982	-3.863612	3.603930
C	1.992687	-2.715656	6.094496
H	2.486052	-2.012627	6.778206
H	2.690548	-3.536302	5.899340
H	1.109958	-3.137950	6.592129
C	2.872245	-1.433888	4.102929
H	3.366340	-0.718913	4.771361
H	2.627712	-0.921871	3.164866
H	3.580123	-2.239335	3.874355
C	-1.534593	1.962860	4.336609
H	-0.930731	2.400200	3.538295
H	-2.446772	1.538949	3.896871
C	-1.866397	2.945203	5.471488
H	-1.022663	3.625708	5.640270
H	-2.750313	3.548126	5.244682
C	-2.065857	2.018024	6.691371
H	-3.063517	1.564066	6.664804
H	-1.956358	2.534929	7.648784
C	-0.988973	0.929673	6.502752
H	-0.046759	1.197381	7.002614
H	-1.317326	-0.050039	6.873670
C	0.003431	-0.346726	0.085830
C	0.730791	0.650916	0.186213
C	1.605972	1.824047	-0.027902
H	1.129696	2.712220	0.407214
H	2.546539	1.676095	0.518123
C	-0.816134	-1.492972	-0.364477
H	-1.835265	-1.382712	0.027796
H	-0.413044	-2.416344	0.071238
C	1.901447	2.066971	-1.530869
H	2.550068	2.943664	-1.631033
H	0.977821	2.253686	-2.088118
H	2.411575	1.206164	-1.975022
C	-0.855091	-1.613182	-1.910082
H	-1.289567	-0.716317	-2.363198
H	-1.472102	-2.474664	-2.186700
H	0.149788	-1.761342	-2.318483

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C	0.281125	1.458424	-3.950542
C	0.126003	1.484072	-2.409262
C	0.253258	0.136418	-1.813269
C	0.376257	-1.073161	-1.574784

C	0.541643	-2.542377	-1.607396
C	0.943560	-3.057410	-3.012193
Au	0.171903	-0.059406	0.462967
C	0.065303	0.344718	2.498601
N	-1.061669	0.149410	3.200631
C	-2.413418	-0.363143	2.753383
C	-3.037272	0.590891	1.710792
N	1.139261	0.824207	3.162701
C	1.036041	1.170963	4.603277
C	2.432964	1.098145	2.467231
H	2.245155	0.847473	1.418096
C	2.813218	2.589476	2.540152
C	-2.293001	-1.801390	2.202907
C	-3.280783	-0.370609	4.031518
C	3.610601	0.164897	2.890624
H	-1.036625	0.352716	4.196791
H	1.299181	-2.835599	-0.870154
H	-0.398309	-3.012428	-1.291932
H	0.881977	2.146622	-1.970372
H	-0.850950	1.903679	-2.138949
H	1.045599	-4.147313	-2.977176
H	1.899887	-2.627922	-3.329577
H	0.181103	-2.804418	-3.756263
H	-0.487888	0.830100	-4.412297
H	1.266531	1.077904	-4.239846
H	0.175221	2.478017	-4.335619
H	-3.288257	-2.176955	1.936908
H	-1.666209	-1.832998	1.303694
H	-1.856040	-2.470269	2.953595
H	-4.038076	0.233569	1.440232
H	-3.127462	1.605210	2.117478
H	-2.433764	0.634209	0.796503
H	-4.285857	-0.733768	3.792974
H	-2.852284	-1.032598	4.794699
H	-3.375051	0.639512	4.449970
H	3.709284	2.764444	1.934036
H	2.000546	3.206426	2.140595
H	3.032947	2.914418	3.560980
H	1.993454	1.544192	4.954635
H	0.269930	1.941478	4.759331
H	0.781343	0.282739	5.194929
H	4.429594	0.443219	2.210359
O	3.995947	0.492064	4.249114
C	3.337395	-1.325740	2.698461
C	2.732021	-2.106144	3.698566
C	2.495288	-3.470900	3.491436
C	2.863120	-4.076046	2.282814
C	3.475478	-3.308885	1.283592
C	3.711330	-1.944662	1.492514
H	2.461940	-1.651693	4.648643
H	2.028991	-4.061808	4.276401
H	2.685945	-5.137516	2.126028
H	3.785660	-3.773886	0.350872
H	4.204328	-1.359907	0.716913
H	4.759411	-0.069314	4.478082

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C	1.007770	2.108342	-3.828213
C	0.894886	1.848257	-2.304955
C	0.324333	0.519028	-1.997750
C	-0.159486	-0.619522	-2.012183
C	-0.717177	-1.945486	-2.354647
C	-0.738867	-2.203554	-3.882344
Au	0.039689	-0.058763	0.207202
C	0.007812	-0.055575	2.280261
N	-1.127982	-0.213893	2.973157
N	1.123481	0.111580	3.007081
C	-2.553675	-0.271199	2.498346
C	2.558189	0.201733	2.568989
H	-1.030386	-0.321306	3.998223
H	-0.127150	-2.722995	-1.852609
H	-1.734136	-2.020638	-1.948300
H	1.885041	1.928437	-1.838057
H	0.271407	2.621825	-1.838373
H	-1.160819	-3.195799	-4.077139
H	0.272580	-2.169772	-4.301078
H	-1.354181	-1.458783	-4.398284
H	0.023948	2.069770	-4.307896
H	1.657582	1.367710	-4.306527
H	1.435350	3.103144	-3.995744
C	3.388543	0.268962	3.871964
C	2.975588	-1.056267	1.771965
C	2.794287	1.491473	1.745773
C	-3.412728	-0.378803	3.779663
C	-2.931512	1.023427	1.740504
C	-2.787579	-1.523079	1.619203
H	-3.843898	-1.581939	1.328010
H	-2.183859	-1.487634	0.703331
H	-2.526481	-2.434309	2.169984
H	-3.993645	0.994534	1.465931
H	-2.760406	1.900989	2.374527
H	-2.345489	1.139879	0.820660
H	-4.473446	-0.411398	3.505474
H	-3.169595	-1.287531	4.342177
H	-3.245551	0.479525	4.440213
H	4.045780	-1.003701	1.535300
H	2.794826	-1.961566	2.363343
H	2.423416	-1.143997	0.828695
H	4.453025	0.347098	3.622994
H	3.104695	1.134539	4.480136
H	3.239087	-0.632791	4.477336
H	3.853925	1.574615	1.472690
H	2.202725	1.485706	0.821482
H	2.513408	2.375770	2.329447
H	0.993253	0.284036	4.018321
B	-0.318738	0.476134	6.451086
F	0.773975	1.032183	5.678805
F	-0.738861	-0.712872	5.724553
F	-1.379614	1.390071	6.469357
F	0.117445	0.127202	7.719424

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C	0.19594004	1.93376007	-3.96466472
C	0.23205173	1.74939159	-2.42680543
C	-0.38841712	0.47568428	-2.00482713
C	-0.96415134	-0.61955661	-1.91992461
C	-1.67814233	-1.89023722	-2.17736406
C	-1.99373049	-2.08981295	-3.68036425
Au	-0.39320388	-0.07455032	0.21116846
C	-0.11546303	-0.06127839	2.26235316
N	-0.63501661	-1.00364917	3.06480544
N	0.59884628	0.89247929	2.87726988
C	-1.48550228	-2.20554265	2.74144813
C	1.32894296	2.08758056	2.31337860
H	-0.43332989	-0.91591353	4.06190729
H	-1.06812327	-2.72509246	-1.81164240
H	-2.60914115	-1.90290080	-1.59766486
H	1.26924656	1.79070668	-2.07452242
H	-0.29150588	2.58177281	-1.94113106
H	-2.51919139	-3.04187814	-3.81126469
H	-1.07405334	-2.11597742	-4.27428926
H	-2.63345606	-1.28492660	-4.05746512
H	-0.83398446	1.94642918	-4.33692699
H	0.74364803	1.13105764	-4.46981920
H	0.66931485	2.88890999	-4.21475490
C	1.96349367	2.78608160	3.53595808
C	2.43957018	1.63023652	1.34231532
C	0.33349289	3.04829840	1.62599489
C	-1.76234080	-2.88261800	4.10180291
C	-2.82124470	-1.76572703	2.10135620
C	-0.71334798	-3.18084125	1.82499021
H	-1.32755347	-4.06744438	1.62715343
H	-0.46670561	-2.71440848	0.86363704
H	0.22114917	-3.50183385	2.30034782
H	-3.44655438	-2.64608493	1.91056312
H	-3.36629182	-1.08813308	2.76930891
H	-2.65731751	-1.24950002	1.14776041
H	-2.38129484	-3.77332197	3.95168785
H	-0.82629342	-3.19293873	4.58286354
H	-2.29783414	-2.20263627	4.77621017
H	2.97473662	2.50332103	0.95138255
H	3.15652921	0.97719261	1.85423831
H	2.02355494	1.08170667	0.48882679
H	2.51697174	3.67223665	3.20842426
H	1.19288765	3.10777535	4.24793851
H	2.66383711	2.11629156	4.05076138
H	0.86910591	3.92356742	1.24035700
H	-0.17231726	2.56329800	0.78268411
H	-0.43030294	3.38795953	2.33574788
H	0.67603411	0.82250762	3.89313370
B	3.14665921	4.74514967	-2.25516301
F	3.89749710	5.50773249	-1.31963962
F	3.44369284	3.36809386	-2.08942876
F	3.49575816	5.14624518	-3.57531558
F	1.76265679	4.96966970	-2.04637586

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Au	0.03978583	0.04924710	0.15396877
C	0.11309675	0.14444539	-1.93113494
N	1.28191142	0.25935037	-2.59810172
C	2.63246101	0.17917546	-1.91268476
C	2.91686762	1.37381173	-0.98147519
N	-1.03995880	0.07190153	-2.62333457
C	-2.47526547	0.09796054	-2.13893042
C	-2.80423328	-1.18866827	-1.34861923
C	-3.33732778	0.14502171	-3.42059989
C	-2.75555478	1.36777824	-1.30388046
H	3.33986941	0.25796102	-2.73913923
C	2.89454460	-1.18791176	-1.24984711
C	1.36600592	0.46435578	-4.09830671
H	-0.98664731	-0.05038450	-3.63349693
H	-3.85637655	-1.17561999	-1.03938493
H	-2.18521674	-1.27007296	-0.44724961
H	-2.63294517	-2.07790827	-1.96672530
H	-3.81998654	1.40034921	-1.04145240
H	-2.51174389	2.26907632	-1.87893071
H	-2.17713409	1.38332302	-0.37313982
H	-4.39726915	0.15569837	-3.14514457
H	-3.15361010	-0.72822342	-4.05632983
H	-3.12604310	1.05047060	-4.00284357
H	3.94234081	-1.23312761	-0.92765444
H	2.71562657	-2.00757033	-1.95449973
H	2.26213104	-1.34504434	-0.36816139
H	3.95850431	1.32307648	-0.64131419
H	2.27261479	1.36072790	-0.09394339
H	2.76848154	2.32642320	-1.50094650
C	2.08634830	1.78496770	-4.44617026
H	0.34925952	0.57667717	-4.47180297
C	1.97868204	-0.76000860	-4.80648759
H	1.92677418	-0.60866889	-5.89074315
H	1.42390646	-1.67313493	-4.56625024
H	3.03165455	-0.90497909	-4.53741860
H	2.01464195	1.94670004	-5.52816584
H	3.15034742	1.76699887	-4.18487206
H	1.61460710	2.63587039	-3.94195160
C	0.75656443	1.87817928	4.40424949
C	0.80346318	1.73268674	2.86250241
C	0.18312065	0.47108802	2.40285056
C	-0.37486946	-0.63064214	2.30245227
C	-1.04977573	-1.92817431	2.52382081
C	-1.25808679	-2.23024634	4.02955550
H	-0.45767572	-2.72680653	2.06023723
H	-2.01868614	-1.92187185	2.00967397
H	1.84416175	1.76877450	2.51755310
H	0.28894676	2.57986060	2.39281264
H	-1.76264915	-3.19673746	4.13342109
H	-0.29981951	-2.27996237	4.55750742
H	-1.87936464	-1.46187883	4.50201353
H	-0.27688034	1.88350357	4.76683135
H	1.29607185	1.05981170	4.89292580

H	1.22952984	2.82440954	4.68761001
B	-1.49283166	-0.59569575	-7.00099899
F	-0.58178226	-1.10572884	-7.96246678
F	-2.82092465	-0.89398300	-7.40332480
F	-1.33318000	0.81034862	-6.89480037
F	-1.23456355	-1.19792324	-5.73813540

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Au	0.25491911	0.01408833	-0.00755096
C	0.02341220	-0.28040667	-2.05898015
N	0.36008777	0.66215133	-2.96639427
C	1.19016239	1.88095065	-2.60981430
C	0.39817362	2.92648859	-1.80154274
N	-0.51079009	-1.43678781	-2.49871071
C	-1.06719357	-2.62281644	-1.74567428
C	0.03699982	-3.30327231	-0.90614799
C	-1.54871096	-3.59933830	-2.84271870
C	-2.27056624	-2.19894620	-0.87494522
H	1.41268506	2.33076580	-3.57852961
C	2.55181354	1.52285636	-1.98308049
C	0.03281522	0.52513815	-4.43857337
H	-0.57675412	-1.56933798	-3.50297913
H	-0.37548783	-4.18387826	-0.39936221
H	0.43732312	-2.62574486	-0.14290246
H	0.86647669	-3.62564389	-1.54668685
H	-2.68894074	-3.07793719	-0.37005253
H	-3.05462742	-1.74525813	-1.49295006
H	-1.97476955	-1.47223949	-0.10947525
H	-1.96843883	-4.49811379	-2.37915563
H	-0.71654889	-3.90826694	-3.48831150
H	-2.32896909	-3.14106221	-3.46370145
H	3.15643902	2.43384294	-1.90041299
H	3.09541860	0.80347756	-2.60588062
H	2.44805892	1.09723267	-0.97812179
H	1.01494072	3.82317024	-1.66773875
H	0.12787436	2.55094103	-0.80725998
H	-0.52277779	3.21344299	-2.31992828
C	-0.60728995	1.80346920	-5.02005666
H	-0.74996053	-0.23206678	-4.51717302
C	1.25755461	0.04947647	-5.24568026
H	0.96833544	-0.11633733	-6.29038261
H	1.66012913	-0.88900239	-4.84702156
H	2.05701452	0.79990361	-5.23275533
H	-0.96378983	1.57676258	-6.03174750
H	0.09881348	2.63652865	-5.09984830
H	-1.46638528	2.12346211	-4.42074542
C	1.71135036	2.49937645	3.68067314
C	1.48265725	2.10803177	2.19899530
C	0.75592278	0.82713395	2.07088884
C	0.15291786	-0.24034136	2.25640289
C	-0.51067145	-1.43288584	2.82848803
C	-0.50001306	-1.42236564	4.37723581
H	-0.00813660	-2.33559714	2.46050803
H	-1.54470372	-1.47787741	2.46561432
H	2.44758146	2.03681682	1.68299224

H	0.91601761	2.89718229	1.69041487
H	-1.00104924	-2.32498931	4.74338401
H	0.52476507	-1.41341044	4.76304578
H	-1.03062631	-0.54768869	4.76804460
H	0.75895574	2.63068543	4.20559008
H	2.29839885	1.73591366	4.20243324
H	2.26287944	3.44458499	3.71129480
B	4.80464370	4.60368444	1.52575985
F	4.86085372	3.20961880	1.27088293
F	3.45453365	5.02013954	1.63748433
F	5.42957487	5.30477945	0.45758064
F	5.49003400	4.88835277	2.73916253

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C	0.40887809	1.42162087	-4.06326278
C	0.28396112	1.45997052	-2.51943945
C	0.31606977	0.10683461	-1.92347485
C	0.35617775	-1.10779391	-1.68330006
C	0.42006046	-2.58482828	-1.71851134
C	0.73357795	-3.12644251	-3.13582690
Au	0.25354875	-0.08249958	0.35674976
C	0.21858381	0.32434324	2.39725590
N	-0.88257760	0.13285180	3.13995897
C	-2.25458705	-0.34754023	2.71395794
C	-2.87712098	0.62646844	1.68814041
N	1.32625560	0.79092520	3.01458570
C	1.29089581	1.13469329	4.45997584
C	2.58444246	1.06659491	2.25907520
H	2.34196122	0.83865004	1.21577080
C	2.98297605	2.55339182	2.33766267
C	-2.17349676	-1.78447118	2.15128978
C	-3.10801887	-0.34731474	4.00072016
C	3.77628146	0.11796155	2.60043512
H	-0.82623865	0.31317165	4.14229543
H	1.18374664	-2.92751216	-1.00931460
H	-0.53640377	-2.99136261	-1.36647567
H	1.09766617	2.06114791	-2.09543129
H	-0.65174085	1.95566136	-2.23283457
H	0.76229499	-4.22086225	-3.10208459
H	1.70481726	-2.76358712	-3.48932619
H	-0.03625801	-2.82168719	-3.85251200
H	-0.41535057	0.85546805	-4.50993208
H	1.35582254	0.96419476	-4.36953699
H	0.37688537	2.44602297	-4.44889819
H	-3.18061186	-2.13714956	1.89823163
H	-1.56089473	-1.82444397	1.24232285
H	-1.73993440	-2.46715979	2.89139227
H	-3.89109424	0.29230232	1.43711334
H	-2.93730276	1.63958463	2.10312290
H	-2.29314575	0.66405589	0.76088920
H	-4.12273055	-0.68479908	3.76415790
H	-2.68700871	-1.02225542	4.75520960
H	-3.17130852	0.65868187	4.43271921
H	3.85015629	2.73032840	1.69121607
H	2.15764566	3.18405724	1.98864013

H	3.25459264	2.85995303	3.35152779
H	2.26648335	1.49995135	4.76727193
H	0.53619833	1.90784022	4.65246830
H	1.05085796	0.25058067	5.06201701
H	4.56189745	0.40836786	1.88626798
O	4.23173805	0.41032443	3.94522450
C	3.48770112	-1.36642854	2.38665659
C	2.91581853	-2.16546337	3.39187299
C	2.66481411	-3.52450116	3.16466704
C	2.98408780	-4.10518141	1.93040007
C	3.56226629	-3.31933629	0.92511380
C	3.81327446	-1.96107387	1.15453939
H	2.68088074	-1.72956126	4.35976634
H	2.22318336	-4.12928362	3.95329343
H	2.79450482	-5.16211442	1.75763314
H	3.83253748	-3.76451636	-0.02956101
H	4.27812268	-1.36130810	0.37294835
H	4.98352831	-0.18120064	4.13300087
F	-0.58290456	1.59346194	8.35713397
B	-1.51376327	1.13854080	7.38628643
F	-2.73118082	0.78628638	8.02436194
F	-0.98149972	0.00091224	6.71929936
F	-1.75338952	2.17070645	6.44120308

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C	-3.95976756	-1.79633616	-2.08134622
C	-3.16677672	-1.22034872	-0.88143529
C	-1.71080722	-1.16424867	-1.14400662
C	-0.56987488	-1.22307985	-1.62570935
C	0.65076785	-1.40586260	-2.44059924
C	0.33567884	-1.94224571	-3.86058637
Au	-0.31225384	-0.36035314	0.47011893
C	0.58137746	0.45770467	2.15537211
N	-0.01975364	1.40004675	2.90139437
C	-1.37487329	2.05010145	2.74410283
C	-1.45700136	2.82491043	1.40910298
N	1.82238361	0.07314370	2.52034040
C	2.50347406	0.72093935	3.66979036
C	2.59569635	-0.92964640	1.72426211
H	1.90964946	-1.24549244	0.93143186
C	3.83404379	-0.29557103	1.06216947
C	-2.49625884	0.99359638	2.85172478
C	-1.48198211	3.04280611	3.92329140
C	2.94374912	-2.24613338	2.48615221
H	0.48746464	1.75187184	3.70908666
H	1.17444491	-0.44513277	-2.51693890
H	1.32964173	-2.09602520	-1.92475520
H	-3.52868542	-0.21150891	-0.64869148
H	-3.34826551	-1.83071984	0.01151484
H	1.27521095	-2.05438060	-4.41204954
H	-0.31006790	-1.24997451	-4.41118408
H	-0.15613259	-2.91951010	-3.81266021
H	-3.63941157	-2.81817139	-2.31027193
H	-3.82412250	-1.17807234	-2.97493395
H	-5.02534325	-1.81425347	-1.82896764

H	-3.47475601	1.48365138	2.78416647
H	-2.42722354	0.25810929	2.04151438
H	-2.43740190	0.46013563	3.80740197
H	-2.42574662	3.33402164	1.33934294
H	-0.66260514	3.57823740	1.34807038
H	-1.36204537	2.15183413	0.54903712
H	-2.44389940	3.56409503	3.88151192
H	-1.41920037	2.51978203	4.88594105
H	-0.68493064	3.79569517	3.87627932
H	4.33047844	-1.04210217	0.43243327
H	3.53367938	0.54816634	0.43087776
H	4.55980060	0.05766963	1.80003997
H	3.49010283	0.28345406	3.79385249
H	2.60624459	1.80077769	3.49957884
H	1.93915693	0.55272576	4.59540561
H	3.34389065	-2.90454421	1.70204064
O	3.99580725	-1.96284149	3.44510322
C	1.73846388	-2.94350078	3.11839109
C	1.38680458	-2.74975180	4.46516791
C	0.27075871	-3.39902914	5.01042461
C	-0.50764727	-4.25045468	4.21621360
C	-0.15903682	-4.45625075	2.87446724
C	0.95798504	-3.81045640	2.33172268
H	1.99372502	-2.10174019	5.09270926
H	0.01230354	-3.24108275	6.05511592
H	-1.37175223	-4.75663526	4.64089941
H	-0.74951907	-5.12631497	2.25381471
H	1.23445302	-3.98583001	1.29298510
H	4.28040806	-2.81488262	3.82355733
F	4.97780063	-3.74227798	-0.35590958
B	4.02311284	-3.78688591	-1.40639803
F	2.71392968	-3.73347698	-0.85803058
F	4.17802527	-4.99793013	-2.13437830
F	4.22293736	-2.68458584	-2.27441051

4BF_4_c

C	-0.71946359	-3.44428639	-2.44342984
C	-0.17991332	-2.17291571	-1.74176633
C	-0.80323449	-1.95730929	-0.41772006
C	-1.47640939	-2.01284435	0.62165272
C	-2.41494924	-2.35948252	1.71065688
C	-3.22466595	-3.64226359	1.39690240
Au	-0.13348813	-0.18065813	0.83628767
C	0.83544156	1.53200050	1.50164084
N	0.40943324	2.23060490	2.56487082
C	-0.76531461	1.98421992	3.48262046
C	-2.09064162	2.02876317	2.69034778
N	1.92277715	1.99499433	0.84845884
C	2.55062928	3.28379401	1.23741077
C	2.48663836	1.29328847	-0.34364763
H	1.89570044	0.37628164	-0.44454481
C	2.31489343	2.14105815	-1.61856821
C	-0.59460476	0.64346264	4.23172698
C	-0.73467758	3.15074220	4.49505029
C	3.96081729	0.83362645	-0.07222000

H	0.99925717	2.99338472	2.88978599
H	-1.85116720	-2.49404104	2.64159182
H	-3.09972930	-1.51863051	1.87527233
H	0.90733865	-2.25012766	-1.61801556
H	-0.36272926	-1.29364501	-2.37124695
H	-3.90158121	-3.84942713	2.23249965
H	-2.56062676	-4.50321868	1.26596797
H	-3.82252171	-3.51713959	0.48787037
H	-1.79949708	-3.37197714	-2.60882545
H	-0.51403275	-4.33953368	-1.84701095
H	-0.22649681	-3.55262819	-3.41550514
H	-1.42959477	0.50093756	4.92823639
H	-0.58142095	-0.20481772	3.53695190
H	0.34174408	0.63499612	4.80133673
H	-2.93339505	1.90733878	3.38138921
H	-2.19988966	2.98880276	2.17200364
H	-2.14522315	1.22730127	1.94407076
H	-1.55824441	3.04089470	5.20834954
H	0.20706611	3.15772670	5.05794658
H	-0.85075653	4.11511384	3.98458473
H	2.61050323	1.56193632	-2.49903505
H	1.26459896	2.43244142	-1.73362585
H	2.92546014	3.05134345	-1.59719743
H	3.36299937	3.51383426	0.54996840
H	1.81657202	4.09722360	1.18268279
H	2.96029639	3.23145190	2.25228710
H	4.59013610	1.72175557	0.07648875
O	4.01856400	-0.01007191	1.10074251
C	4.52960534	0.04054059	-1.24279208
C	4.13132748	-1.28898362	-1.46951896
C	4.64793355	-2.01239686	-2.55106791
C	5.56848876	-1.41503751	-3.42316488
C	5.97561884	-0.09383997	-3.20071411
C	5.46121912	0.62627068	-2.11452227
H	3.43309148	-1.76664287	-0.78572895
H	4.33665860	-3.04225642	-2.71019299
H	5.97037338	-1.97747723	-4.26271847
H	6.69782678	0.37450590	-3.86501873
H	5.79094083	1.64938723	-1.94207960
H	3.91096855	0.53277076	1.90906228
F	3.11774321	3.05321299	4.70953696
B	4.10641723	2.03981848	4.80105066
F	3.90781548	1.09257093	3.74579589
F	3.99882514	1.37463315	6.04393153
F	5.39202673	2.61742949	4.66884552

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