Supporting Information for

Synthesis and Characterization of *N*-Heterocyclic Carbene-M···OEt_2 Complexes (M = Cu, Ag, Au). Analysis of Solvated Auxiliary-Ligand Free $[(NHC)M]^+$ Species

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Content

Experimental Procedures:

All manipulations were carried out under an atmosphere of purified nitrogen using standard Schlenk techniques or in a MBRAUN LABMaster glovebox equipped with a -10 °C refrigerator. Solvents were purchased from commercial sources, and purified by conventional methods prior to use. Glassware was oven-dried at 150^{o}C overnight. The NMR spectra were recorded at the room temperature on a JEOL Eclipse 500 spectrometer (^{1}H: 500.16 MHz, ^{13}C: 125.77 MHz and 470.62 MHz) and a JEOL Eclipse 300 spectrometer (^{19}F: 282.78 MHz). Chemical shifts for ^{1}H and ^{13}C spectra are referenced to the solvent peak (^{1}H; CD_2Cl_2, δ 5.32, ^{13}C; CD_2Cl_2, δ 53.84, $CDCl_3$, δ 7.26, ^{13}C; $CDCl_3$, δ 77.16, ^{1}H; D_6-dmso, δ 2.50, ^{13}C; D_6-dmso, δ 39.52.) IR spectra were collected at room temperature on a Shimadzu IRPrestige-21 FTIR containing an ATR attachment at 2 cm^{-1} resolution. Elemental analyses were performed at Intertek USA, Whitehouse, NJ. Deuterated solvents were purchased from Acros Organics and Cambridge Isotope Laboratories, respectively. Deuterated solvents were purchased from Acros Organics and Cambridge Isotope Laboratories, respectively. (SIPr)CuCl,[1] (SIPr)AgCl,[2] (SIPr)AuCl,[3] (^{Et2}CAAC)CuCl,[4] (^{Et2}CAAC)AgCl,[5] (^{Et2}CAAC)AuCl[4] were prepared according to literature procedures.

[(SIPr)Cu(OEt$_2$)][SbF$_6$] (1): A mixture of (SIPr)CuCl (0.120 g, 0.245 mmol) and $AgSbF_6$ (0.084 g, 0.245 mmol) in a mixed solvent dichloromethane/diethylether (5:1; 12 mL) was stirred for 45 minutes at 0 °C. The resulting mixture was filtered through a pad of Celite *via* canula and the filtrate was concentrated to ~3 mL under reduced pressure. The concentrated solution was layered with hexane (3 mL) and kept in refrigerator at -20 °C to obtain colorless crystals of [(SIPr)Cu(OEt$_2$)][SbF_6] (78 % yield). ^{1}H NMR (CD_2Cl_2, 500.16 MHz, 298 K): δ 7.45 (t, 2H, $^{3}J_{HH}$ = 8 Hz, $C_6\underline{H}_3$), 7.30 (d, 4H, $^{3}J_{HH}$ = 8 Hz, $C_6\underline{H}_3$), 4.18 (s, 4H, $C\underline{H}_2$), 3.48 (q, 4H, $^{3}J_{HH}$ = 6.9

Hz, OC$\underline{H}_2$CH$_3$), 3.05 (sept, 4H, $^3J_{HH}$ = 6.9 Hz, C$\underline{H}$(CH$_3$)$_2$), 1.37 (d, 12H, $^3J_{HH}$ = 6.9 Hz, CH(C$\underline{H}_3$)$_2$), 1.30 (d, 12H, $^3J_{HH}$ = 6.9 Hz, CH(C$\underline{H}_3$)$_2$), 0.51 (t, 6H, OCH$_2$C$\underline{H}_3$). ^{13}C{^{1}H} NMR (CD$_2$Cl$_2$, 125.77 MHz, 298 K): δ 199.7 (Cu–N$\underline{C}$N), 147.2, 134.3, 130.8, 125.2, 72.4 (br), 54.3, 29.2, 25.7, 24.1, 14.9. Anal. Calcd. for $C_{31}H_{48}N_2OF_6CuSb$: C, 48.73; H, 6.33; N, 3.67. Found: C, 48.26; H, 6.27; N, 3.20.

[(SIPr)Ag(OEt$_2$)][SbF$_6$] (2): A mixture of (SIPr)AgCl (0.180 g, 0.336 mmol) and AgSbF$_6$ (0.128 g, 0.372 mmol) in a mixed solvent dichloromethane/diethylether (5:1; 12 mL) was stirred for 45 minutes at 0 °C. The resulting mixture was filtered through a pad of Celite *via* canula and the filtrate was concentrated to ~3 mL under reduced pressure. The concentrated solution was layered with hexane (3 mL) and kept in refrigerator at -20 °C to obtain colorless crystals of [(SIPr)Ag(OEt$_2$)][SbF$_6$] (0.190 g, 70% yield). ^{1}H NMR (CD$_2$Cl$_2$, 500.16 MHz, 298 K): δ 7.46 (t, 2H, $^3J_{HH}$ = 8 Hz, C$_6\underline{H}_3$), 7.30 (d, 4H, $^3J_{HH}$ = 8 Hz, C$_6\underline{H}_3$), 4.24 (s, 4H, C$\underline{H}_2$), 3.47 (q, 4H, $^3J_{HH}$ = 6.9 Hz, OC$\underline{H}_2$CH$_3$), 3.06 (sept, 4H, $^3J_{HH}$ = 6.9 Hz, C$\underline{H}$(CH$_3$)$_2$), 1.37 (d, 12H, $^3J_{HH}$ = 6.9 Hz, CH(C$\underline{H}_3$)$_2$), 1.29 (d, 12H, $^3J_{HH}$ = 6.9 Hz, CH(C$\underline{H}_3$)$_2$), 0.76 (t, 6H, OCH$_2$C$\underline{H}_3$). ^{13}C{^{1}H} NMR (CD$_2$Cl$_2$, 125.77 MHz, 298 K): δ 146.9, 134.2, 130.3, 124.8, 69.3 (br), 53.9, 28.8, 25.4, 23.8, 15.5. Anal. Calcd. for $C_{31}H_{48}N_2OF_6AgSb$: C, 46.06; H, 5.99; N, 3.47. Found: C, 45.60; H, 5.99; N, 3.01.

[(^{Et2}CAAC)M(OEt$_2$)][SbF$_6$]: A mixture of (^{Et2}CAAC)MCl [M= Cu (124 mg), Ag (137 mg), Au (164 mg); 0.3 mmol] and AgSbF$_6$ (103 mg, 0.3 mmol) in a mixed solvent dichloromethane/diethyl ether (1:1; 6 mL) was stirred for 45 minutes at room temperature. The resulting mixture was filtered and the filtrate was layered with Et$_2$O (3 mL) overnight to obtain colorless crystals.

[(^{Et2}CAAC)Cu(OEt$_2$)][SbF$_6$] (4): 130 mg, 63 % yield. ^{1}H NMR (CD_2Cl_2, 500.16 MHz, 298 K): δ 7.48 (t, 1H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 7.35 (d, 2H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 3.66 (q, 4H, J_{HH} = 6.9 Hz, $OC\underline{H}_2CH_3$), 2.85 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}(CH_3)_2$), 2.1 (s, 2H, $C\underline{H}_2$), 1.85 (m, 2H, $C\underline{H}_2CH_3$), 1.72 (m, 2H, $C\underline{H}_2CH_3$), 1.44 (s, 6H, $C(C\underline{H}_3)_2$), 1.34 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.22 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.08 (t, 6H, J_{HH} = 7.4 Hz, $CH(C\underline{H}_3)_2$), 1.00 (t, 6H, J_{HH} = 7.4 Hz, $OCH(C\underline{H}_3)_2$). $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 125.77 MHz, 298 K): δ 247.0 (Cu–$\underline{C}$), 144.9, 135.4, 130.5, 125.5, 82.3, 71.8, 62.4, 42.1, 30.9, 29.2, 27.0, 22.2, 15.2, 9.3.

^{1}H NMR (acetone-d_6, 500.16 MHz, 298 K): δ 7.51(t, 1H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 7.44 (d, 2H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 3.39 (q, 4H, J_{HH} = 6.9 Hz, $OC\underline{H}_2CH_3$), 3.02 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}(CH_3)_2$), 2.18 (s, 2H, $C\underline{H}_2$), 1.95 (m, 2H, $C\underline{H}_2CH_3$), 1.87 (m, 2H, $C\underline{H}_2CH_3$), 1.49 (s, 6H, $C(C\underline{H}_3)_2$), 1.35 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.23 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.10 (overlapped t, 12H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$ and $OCH(C\underline{H}_3)_2$). $^{13}C\{^1H\}$ NMR (acetone-d_6, 125.77 MHz, 298 K): δ 250.2 (Cu–$\underline{C}$), 146.0, 136.6, 130.8, 126.0, 82.7, 76.0, 63.3, 42.6, 31.4, 29.2, 27.0, 22.2, 15.2, 9.7. Anal. Calcd. for $C_{26}H_{45}NOF_6CuSb$: C, 45.46; H, 6.60; N, 2.04. Found: C, 45.86; H, 6.72; N, 2.31.

[(^{Et2}CAAC)Ag(OEt$_2$)][SbF$_6$] (5): 151 mg, 69% yield. ^{1}H NMR (CD_2Cl_2, 500.16 MHz, 298 K): δ 7.46 (t, 1H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 7.33 (t, 1H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 7.30 (d, 2H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 7.17 (d, 2H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 3.53 (q, 4H, J_{HH} = 6.9 Hz, $OC\underline{H}_2CH_3$), 2.81 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}(CH_3)_2$), 2.63 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}(CH_3)_2$), 2.1 (s, 2H, $C\underline{H}_2$), 1.94 (s, 2H, $C\underline{H}_2$), 1.84 (m, 2H, $C\underline{H}_2CH_3$), 1.68 (m, 4H, $C\underline{H}_2CH_3$), 1.48 (m, 2H, $C\underline{H}_2CH_3$), 1.44 (s, 6H, $C(C\underline{H}_3)_2$), 1.31 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.29 (s, 6H, $C(C\underline{H}_3)_2$), 1.21 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.10 (d, 6H, J_{HH} = 6.9 Hz, $CH(C\underline{H}_3)_2$), 1.04 (t, 6H, J_{HH} = 7.4 Hz, $CH(C\underline{H}_3)_2$), 0.90 (t, 6H, J_{HH} = 7.4 Hz, $CH(C\underline{H}_3)_2$), 0.76 (t, 6H, J_{HH} = 7.4 Hz, $OCH(C\underline{H}_3)_2$). $^{13}C\{^1H\}$ NMR (CD_2Cl_2,

125.77 MHz, 298 K): δ 145.0, 135.1, 130.3, 125.4, 84.1, 68.2, 62.6, 41.8, 31.7, 29.5, 27.6, 22.4, 15.9, 9.8. Anal. Calcd. for $C_{26}H_{45}NOF_6AgSb$: C, 42.70; H, 6.20; N, 1.92. Found: C, 43.81; H, 6.45; N, 1.97.

[(^{Et2}CAAC)Au(OEt$_2$)][SbF$_6$] (6): 202 mg, 82 % yield. ^{1}H NMR ($CDCl_3$, 500.16 MHz, 298 K): δ 7.47 (t, 1H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 7.30 (d, 2H, J_{HH} = 8 Hz, $C_6\underline{H}_3$), 3.89 (q, 4H, J_{HH} = 6.9 Hz, $OC\underline{H}_2CH_3$), 2.76 (sept, 2H, $^3J_{HH}$ = 6.9 Hz, $C\underline{H}(CH_3)_2$), 2.2 (s, 2H, $C\underline{H}_2$), 1.88 (m, 2H, $C\underline{H}_2CH_3$), 1.75 (m, 2H, $C\underline{H}_2CH_3$), 1.46 (s, 6H, $C(C\underline{H}_3)_2$), 1.34-1.25 (m, 12H, $CH(C\underline{H}_3)_2$), 1.13-1.07 (m, 12H, $CH(C\underline{H}_3)_2$ and $OCH(C\underline{H}_3)_2$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 125.77 MHz, 298 K): δ 224.7(Au–$\underline{C}$), 144.9, 135.0, 130.8, 125.6, 82.0, 72.8, 61.9, 41.2, 31.7, 29.3, 27.1, 22.8, 15.5, 9.4. Anal. Calcd. for $C_{26}H_{45}NOF_6AuSb$: C, 38.07; H, 5.53; N, 1.71. Found: C, 38.41; H, 5.64; N, 1.67.

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 compounds [(SIPr)Cu(OEt$_2$)][SbF$_6$] (**1**), [(SIPr)Ag(OEt$_2$)][SbF$_6$] (**2**), [(^{Et2}CAAC)Ag(OEt$_2$)][SbF$_6$] (**5**), and [(^{Et2}CAAC)Au(OEt$_2$)][SbF$_6$] (**6**) and were measured at 100(2) K on a Bruker D8 Quest with a Photon 100 CMOS detector equipped with an Oxford Cryosystems 700 series cooler, a Triumph monochromator, and a Mo Kα fine-focus sealed tube (λ = 0.71073 Å). Intensity data were processed using the Bruker ApexII program suite. Absorption corrections were applied by using SADABS.[6] Initial atomic positions were located by direct methods using XT,[7] and the structures of the compounds were refined by the least-squares method using SHELXL.[8] All the non-hydrogen atoms were refined anisotropically. All

hydrogen atoms were placed at calculated positions and refined using a riding model. X-ray structural figures were generated using Olex2.[9] Compounds **1** and **2** are isomorphous. They crystallize with two molecules of CH_2Cl_2 in the asymmetric unit. Compound **5** crystallizes in $P2_1/c$ space group with three chemically similar molecules in the asymmetric unit. The CCDC 2016681-2016684 contain the supplementary crystallographic data of **1, 2, 5** and **6,** deposited at the Cambridge Crystallographic Data Centre. X-ray crystal structural data of the water adducts, [(SIPr)Cu(OH_2)][SbF_6] (**7**), [(^{Et2}CAAC)Cu(OH_2)][SbF_6] (**10**), and [(^{Et2}CAAC)Au(OH_2)][SbF_6] (**12**) have also been determined, and CCDC 2016685-2016687 contain the supplementary crystallographic data. These detailed data files can be obtained free of charge *via* http://www.ccdc.cam.ac.uk/conts/retrieving.html or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge, CB2 1EZ, UK).

Table S1. Selected bond distances (Å) and angles (°) of NHC supported coinage metal water adducts

Compound	**M-O**	**M-C**	**O-M-C**
[(SIPr)Cu(OH_2)][SbF_6] (**7**)	1.902(5)	1.876(5)	167.5(2)
Calculated	*1.976*	*1.869*	*179.8*
[(^{Et2}CAAC)Au(OH_2)][SbF_6] (**10**)	1.8856(10)	1.8753(12)	178.70(5)
Calculated	*1.998*	*1.860*	*179.3*
[(^{Et2}CAAC)Au(OH_2)][SbF_6] (**12**)	2.0889(15)	1.957(2)	177.68(7)
Calculated	*2.206*	*1.977*	*178.4*

References

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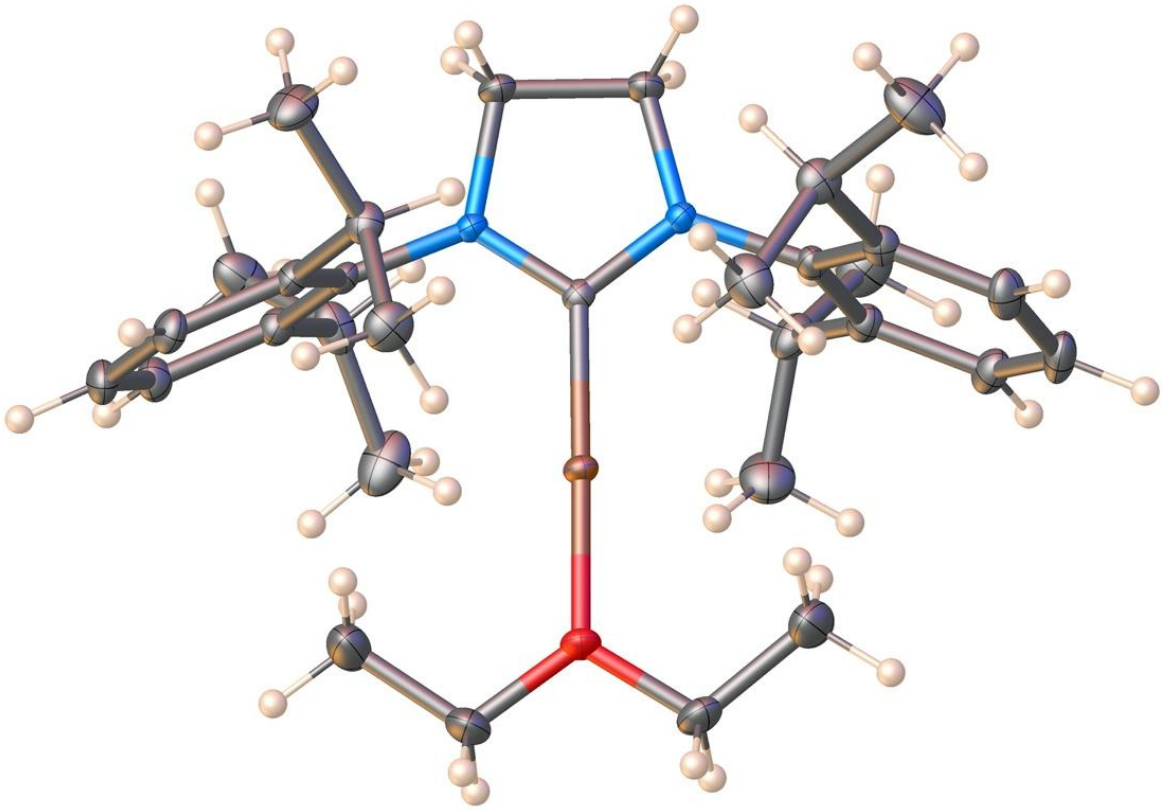

Figure S1. Molecular structures of [(SIPr)Cu(OEt_2)][SbF_6]. The $[SbF_6]^-$ counter ion has been omitted for clarity.

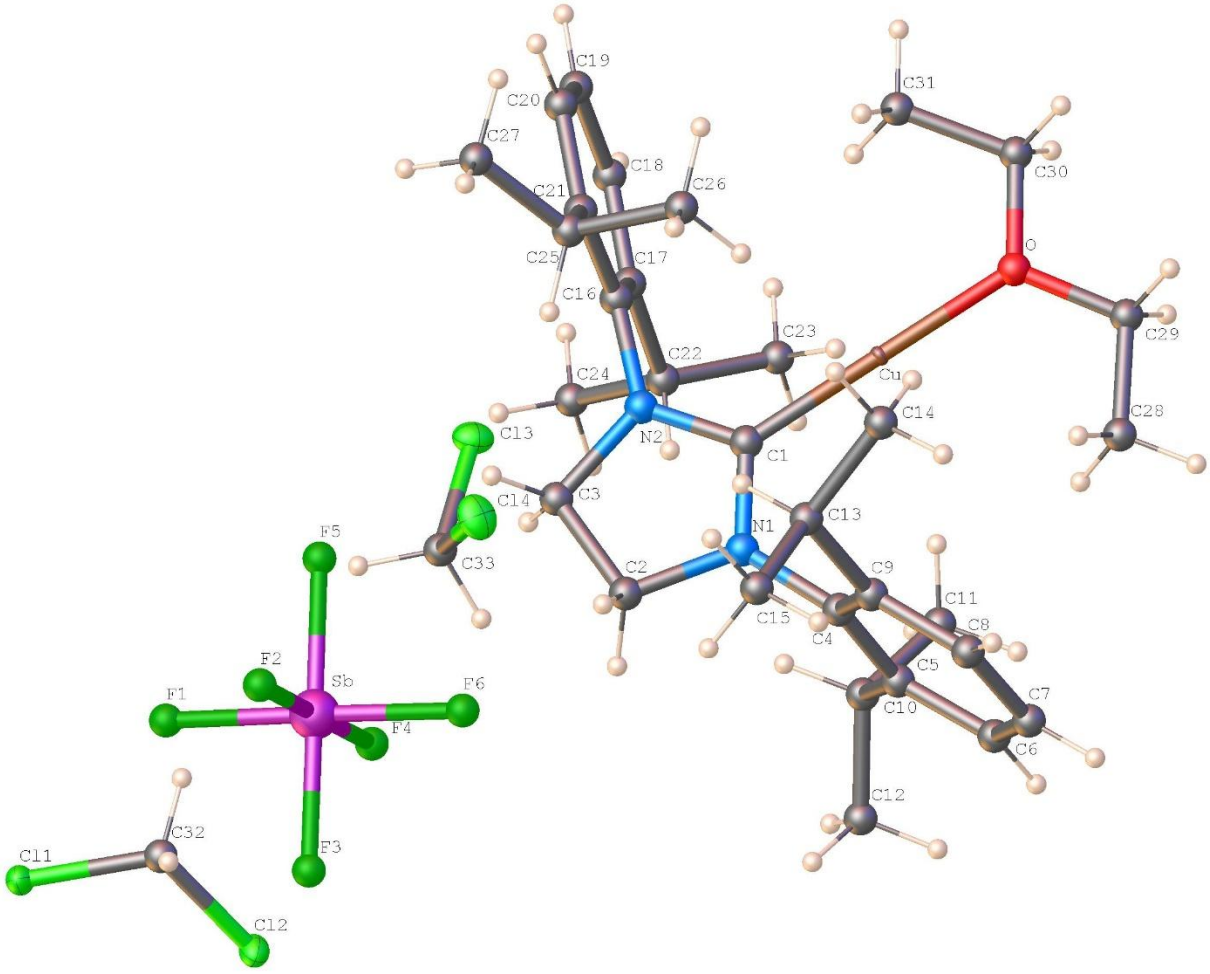

Figure S2. Molecules in the asymmetric unit of [(SIPr)Cu(OEt_2)][SbF_6].

Table S2. Crystal data and structure refinement for [(SIPr)Cu(OEt$_2$)][SbF$_6$]•2CH$_2$Cl$_2$

Empirical formula	$C_{33}H_{52}Cl_4CuF_6N_2OSb$
Formula weight	933.85
Temperature/K	100.01
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.0397(6)
b/Å	12.0879(4)
c/Å	21.5503(7)
α/°	90
β/°	113.0470(10)
γ/°	90
Volume/Å^3	4084.5(2)
Z	4
ρ_{calc}g/cm^3	1.519
μ/mm^{-1}	1.499
F(000)	1896.0
Crystal size/mm^3	0.25 × 0.24 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.674 to 61.156
Index ranges	$-24 \leq h \leq 24$, $-17 \leq k \leq 17$, $-30 \leq l \leq 30$
Reflections collected	54257
Independent reflections	12526 [R_{int} = 0.0299, R_{sigma} = 0.0259]
Data/restraints/parameters	12526/0/443
Goodness-of-fit on F^2	1.016
Final R indexes [I>=2σ (I)]	R_1 = 0.0280, wR_2 = 0.0620
Final R indexes [all data]	R_1 = 0.0373, wR_2 = 0.0655
Largest diff. peak/hole / e Å^{-3}	1.10/-1.10

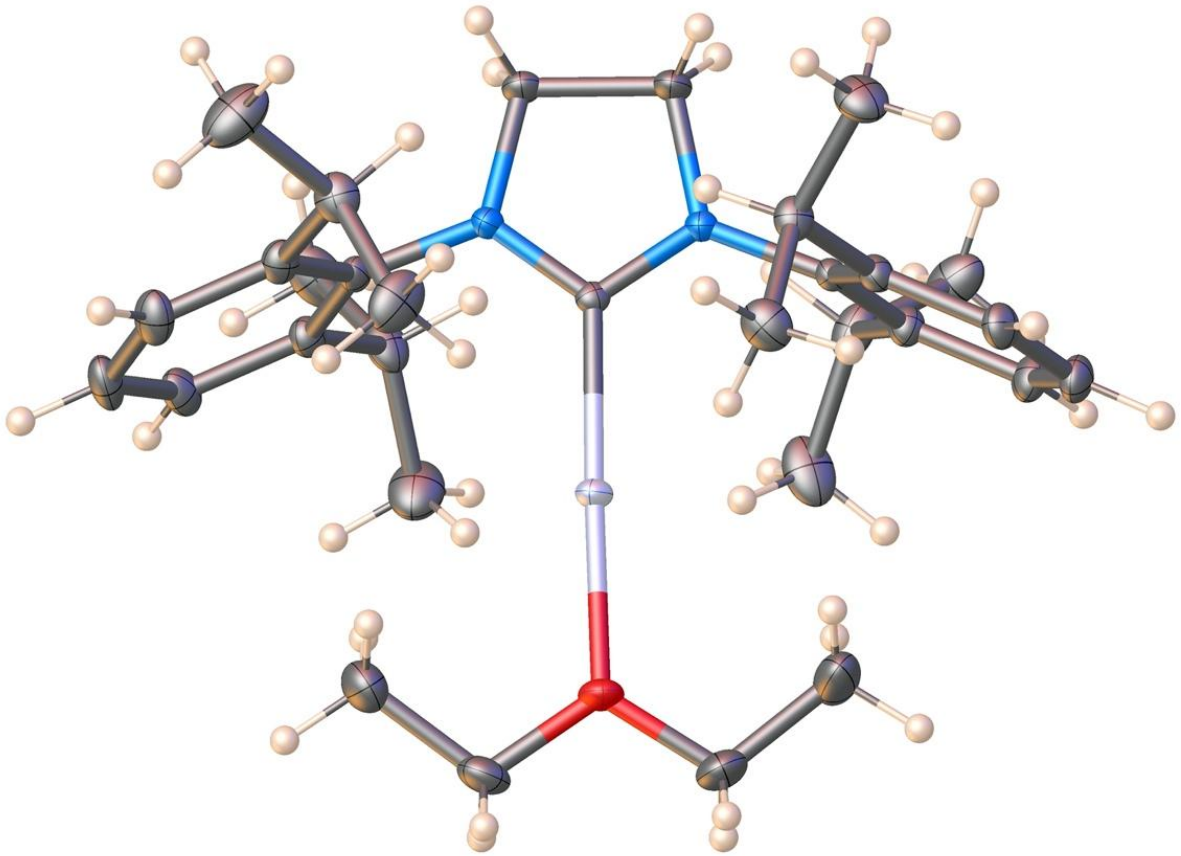

Figure S3. Molecular structures of [(SIPr)Ag(OEt_2)][SbF_6]. The [SbF_6]$^-$ counter ion has been omitted for clarity.

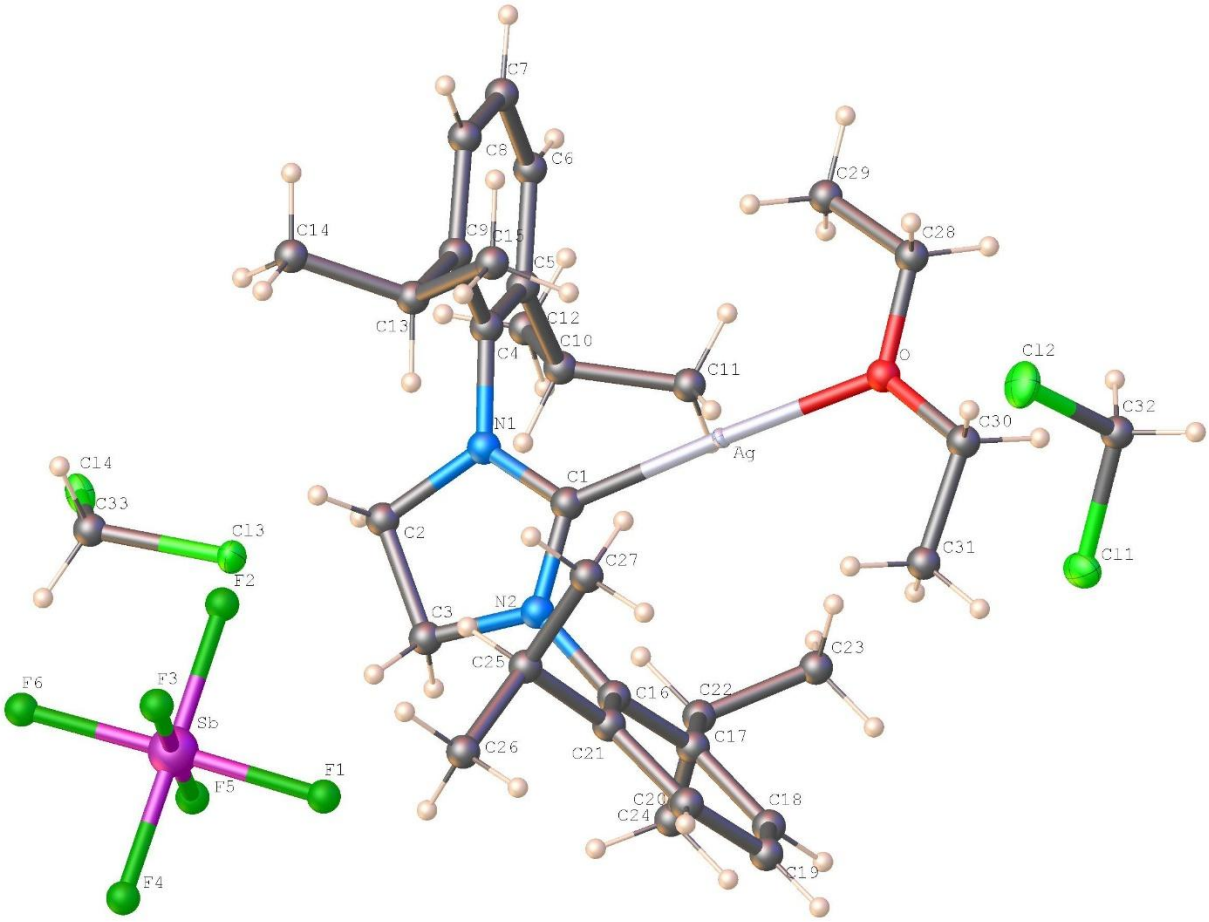

Figure S4. Molecules in the asymmetric unit of [(SIPr)Ag(OEt_2)][SbF_6].

Table S3. Crystal data and structure refinement for [(SIPr)Ag(OEt$_2$)][SbF$_6$]•2CH$_2$Cl$_2$

Empirical formula	$C_{33}H_{52}AgCl_4F_6N_2OSb$
Formula weight	978.18
Temperature/K	100.25
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.0105(7)
b/Å	12.2904(5)
c/Å	21.5411(9)
α/°	90
β/°	113.2430(10)
γ/°	90
Volume/Å^3	4138.0(3)
Z	4
ρ_{calc}g/cm^3	1.570
μ/mm^{-1}	1.439
F(000)	1968.0
Crystal size/mm^3	0.36 × 0.3 × 0.26
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.826 to 61.016
Index ranges	$-24 \leq h \leq 24$, $-17 \leq k \leq 17$, $-30 \leq l \leq 30$
Reflections collected	56604
Independent reflections	12609 [R_{int} = 0.0215, R_{sigma} = 0.0187]
Data/restraints/parameters	12609/0/443
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0222, wR_2 = 0.0537
Final R indexes [all data]	R_1 = 0.0254, wR_2 = 0.0552
Largest diff. peak/hole / e Å^{-3}	1.34/-1.15

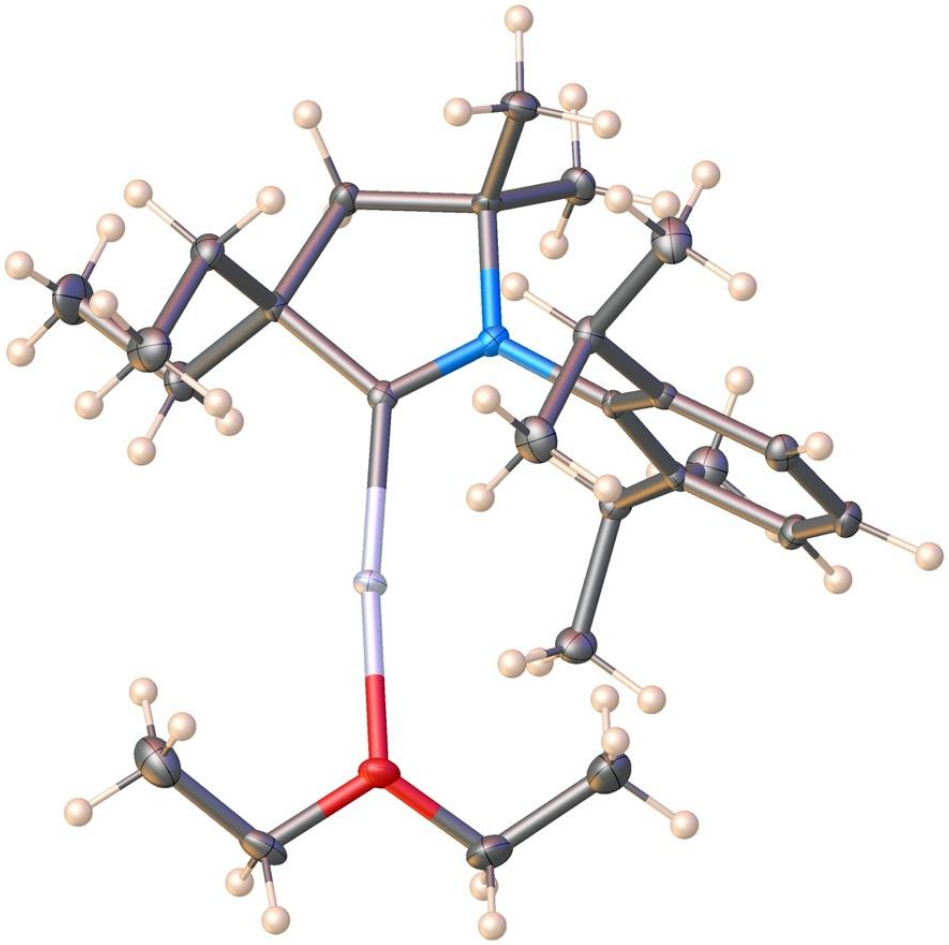

Figure S5. Molecular structures of [(^{Et2}CAAC)Ag(OEt_2)][SbF_6]. The [SbF_6]$^-$ counter ion has been omitted for clarity.

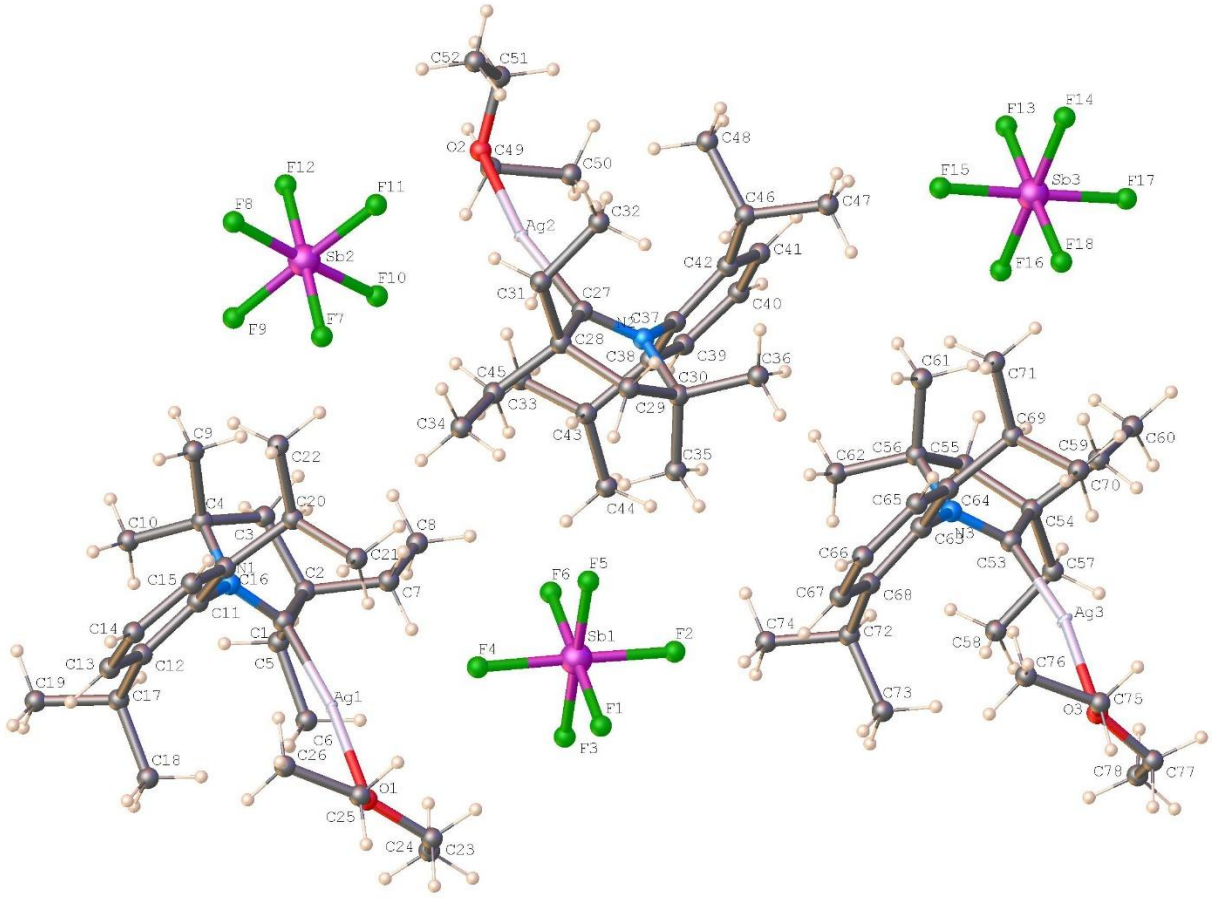

Figure S6. Molecules in the asymmetric unit of [(^{Et2}CAAC)Ag(OEt_2)][SbF_6].

Table S4. Crystal data and structure refinement for [(^{Et2}CAAC)Ag(OEt_2)][SbF_6]

Empirical formula	$C_{26}H_{45}AgF_6NOSb$
Formula weight	731.25
Temperature/K	100.01
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.0885(4)
b/Å	41.0903(15)
c/Å	21.5549(8)
α/°	90
β/°	93.0160(10)
γ/°	90
Volume/Å^3	8923.0(6)
Z	12
ρ_{calc}g/cm^3	1.633
μ/mm^{-1}	1.623
F(000)	4416.0
Crystal size/mm^3	0.3 × 0.13 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.744 to 54.97
Index ranges	$-13 \leq h \leq 13$, $-53 \leq k \leq 53$, $-27 \leq l \leq 27$
Reflections collected	100629
Independent reflections	20413 [R_{int} = 0.0323, R_{sigma} = 0.0239]
Data/restraints/parameters	20413/0/1003
Goodness-of-fit on F^2	1.108
Final R indexes [I>=2σ (I)]	R_1 = 0.0319, wR_2 = 0.0710
Final R indexes [all data]	R_1 = 0.0396, wR_2 = 0.0737
Largest diff. peak/hole / e Å^{-3}	2.59/-1.18

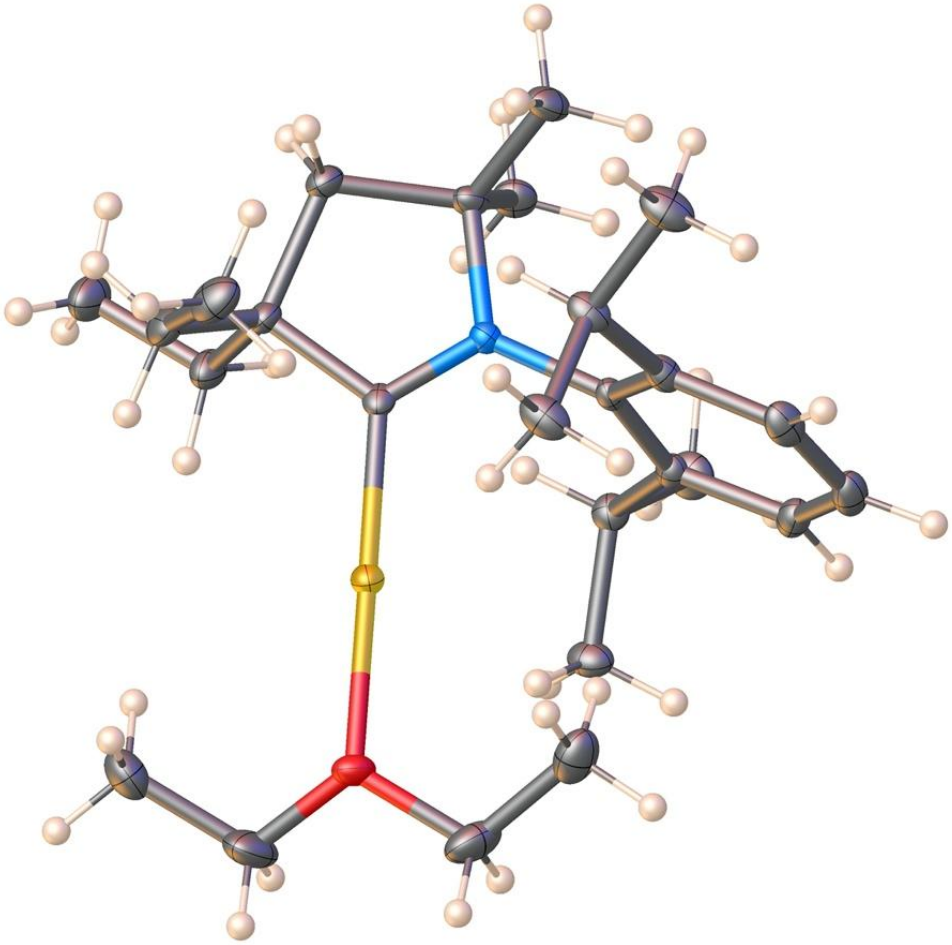

Figure S7. Molecular structures of [(^{Et2}CAAC)Au(OEt_2)][SbF_6]. The [SbF_6]$^-$ counter ion has been omitted for clarity.

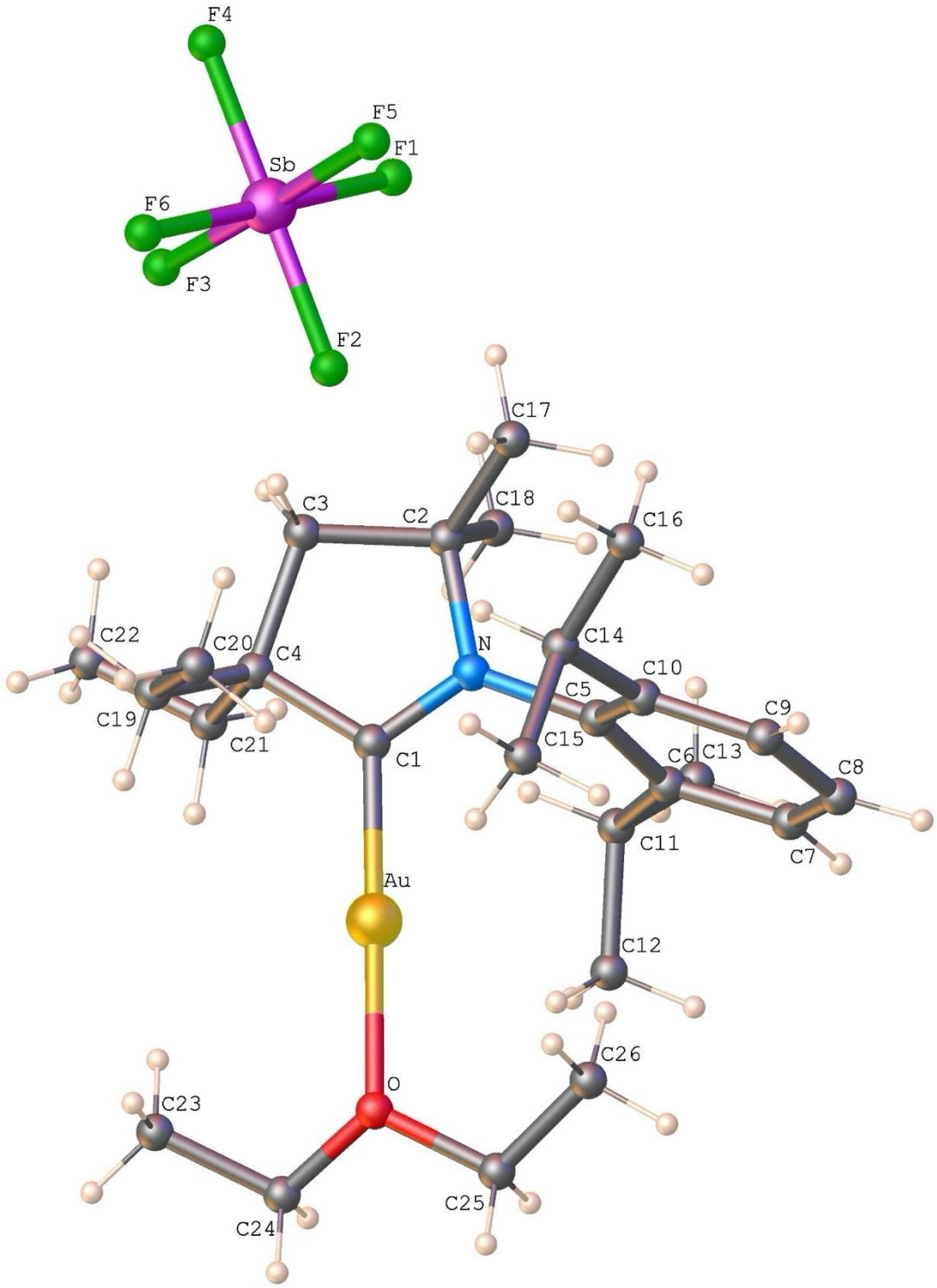

Figure S8. Asymmetric unit of [(^{Et2}CAAC)Au(OEt$_2$)][SbF$_6$].

Table S5. Crystal data and structure refinement for [(^{Et2}CAAC)Au(OEt$_2$)][SbF$_6$].

Empirical formula	$C_{26}H_{45}AuF_6NOSb$
Formula weight	820.34
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.5000(7)
b/Å	17.3023(10)
c/Å	14.9126(9)
α/°	90
β/°	96.383(2)
γ/°	90
Volume/Å^3	2948.9(3)
Z	4
ρ_{calc}g/cm^3	1.848
μ/mm^{-1}	5.942
F(000)	1600.0
Crystal size/mm^3	0.31 × 0.31 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.452 to 66.49
Index ranges	$-17 \leq h \leq 17$, $-26 \leq k \leq 26$, $-23 \leq l \leq 22$
Reflections collected	70958
Independent reflections	11301 [R_{int} = 0.0368, R_{sigma} = 0.0246]
Data/restraints/parameters	11301/0/336
Goodness-of-fit on F^2	1.100
Final R indexes [I>=2σ (I)]	R_1 = 0.0256, wR_2 = 0.0543
Final R indexes [all data]	R_1 = 0.0308, wR_2 = 0.0560
Largest diff. peak/hole / e Å^{-3}	1.94/-1.50

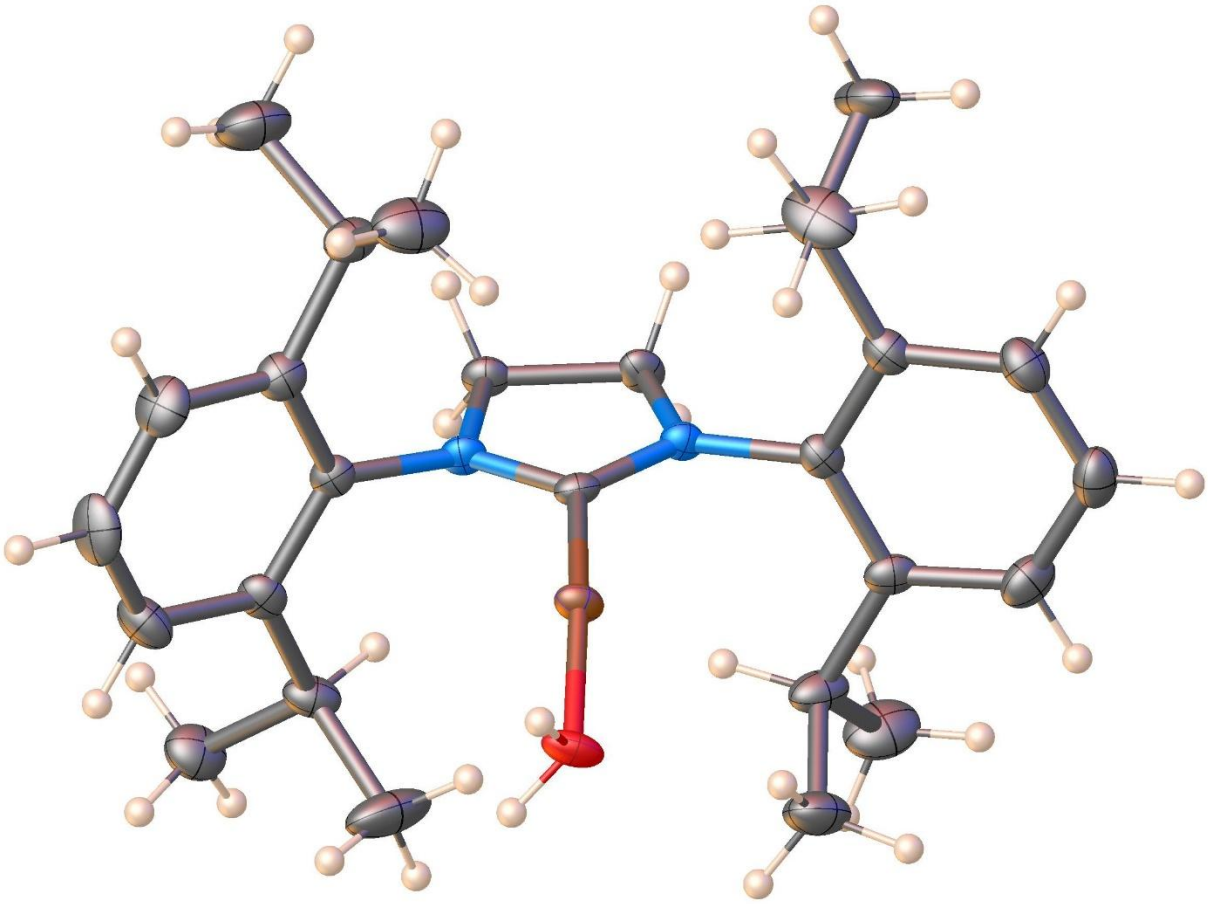

Figure S9. Molecular structures of [(SIPr)Cu(OH_2)][SbF_6]. The $[SbF_6]^-$ counter ion has been omitted for clarity.

Table S6. Crystal data and structure refinement for [(SIPr)Cu(OH_2)][SbF_6]•0.5(H_2O).

Empirical formula	$C_{27}H_{41}CuF_6N_2O_{1.5}Sb$
Formula weight	716.91
Temperature/K	100.0
Crystal system	trigonal
Space group	R3c
a/Å	27.8000(10)
b/Å	27.8000(10)
c/Å	21.5997(8)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	14456.7(12)
Z	18
ρ_{calc}g/cm^3	1.482
μ/mm^{-1}	1.560
F(000)	6534.0
Crystal size/mm^3	0.41 × 0.09 × 0.09
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.854 to 56.558
Index ranges	$-37 \leq h \leq 37$, $-37 \leq k \leq 37$, $-28 \leq l \leq 28$
Reflections collected	56564
Independent reflections	7972 [R_{int} = 0.0424, R_{sigma} = 0.0280]
Data/restraints/parameters	7972/0/360
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0377, wR_2 = 0.0960
Final R indexes [all data]	R_1 = 0.0412, wR_2 = 0.0982
Largest diff. peak/hole / e Å^{-3}	1.85/-0.79

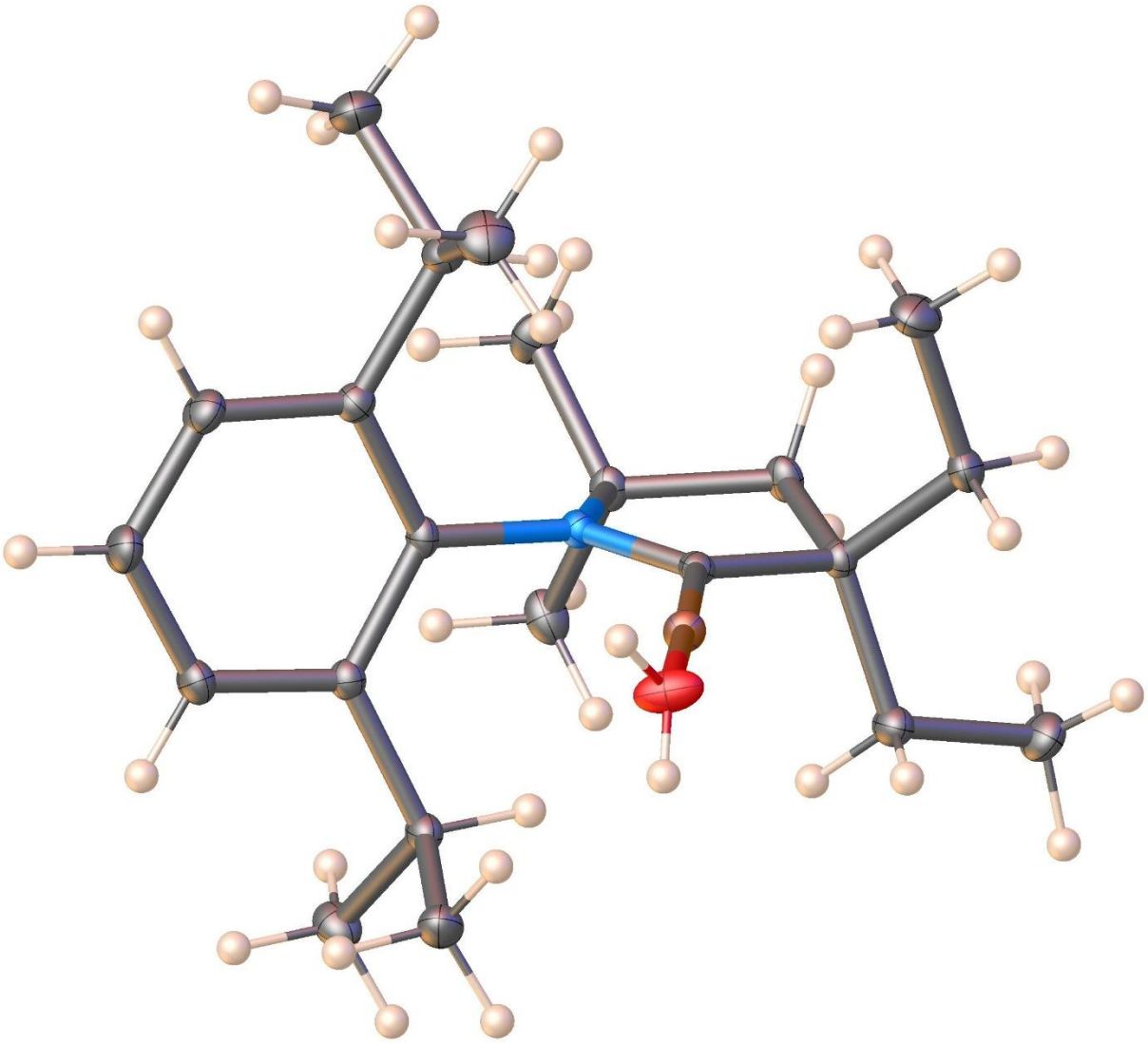

Figure S10. Molecular structures of [(^{Et2}CAAC)Cu(OH_2)][SbF_6]. The [SbF_6]$^-$ counter ion has been omitted for clarity.

Table S7 Crystal data and structure refinement for [(^{Et2}CAAC)Cu(OH$_2$)][SbF$_6$].

Empirical formula	$C_{22}H_{37}CuF_6NOSb$
Formula weight	630.81
Temperature/K	99.99
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.4439(3)
b/Å	11.1960(4)
c/Å	27.3426(10)
α/°	90
β/°	97.2270(10)
γ/°	90
Volume/Å^3	2564.38(16)
Z	4
ρ_{calc}g/cm^3	1.634
μ/mm^{-1}	1.940
F(000)	1272.0
Crystal size/mm^3	0.32 × 0.28 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.792 to 61.016
Index ranges	$-12 \leq h \leq 12$, $-15 \leq k \leq 15$, $-39 \leq l \leq 39$
Reflections collected	34846
Independent reflections	7793 [R_{int} = 0.0219, R_{sigma} = 0.0185]
Data/restraints/parameters	7793/0/306
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0194, wR_2 = 0.0449
Final R indexes [all data]	R_1 = 0.0216, wR_2 = 0.0457
Largest diff. peak/hole / e Å^{-3}	0.49/-0.41

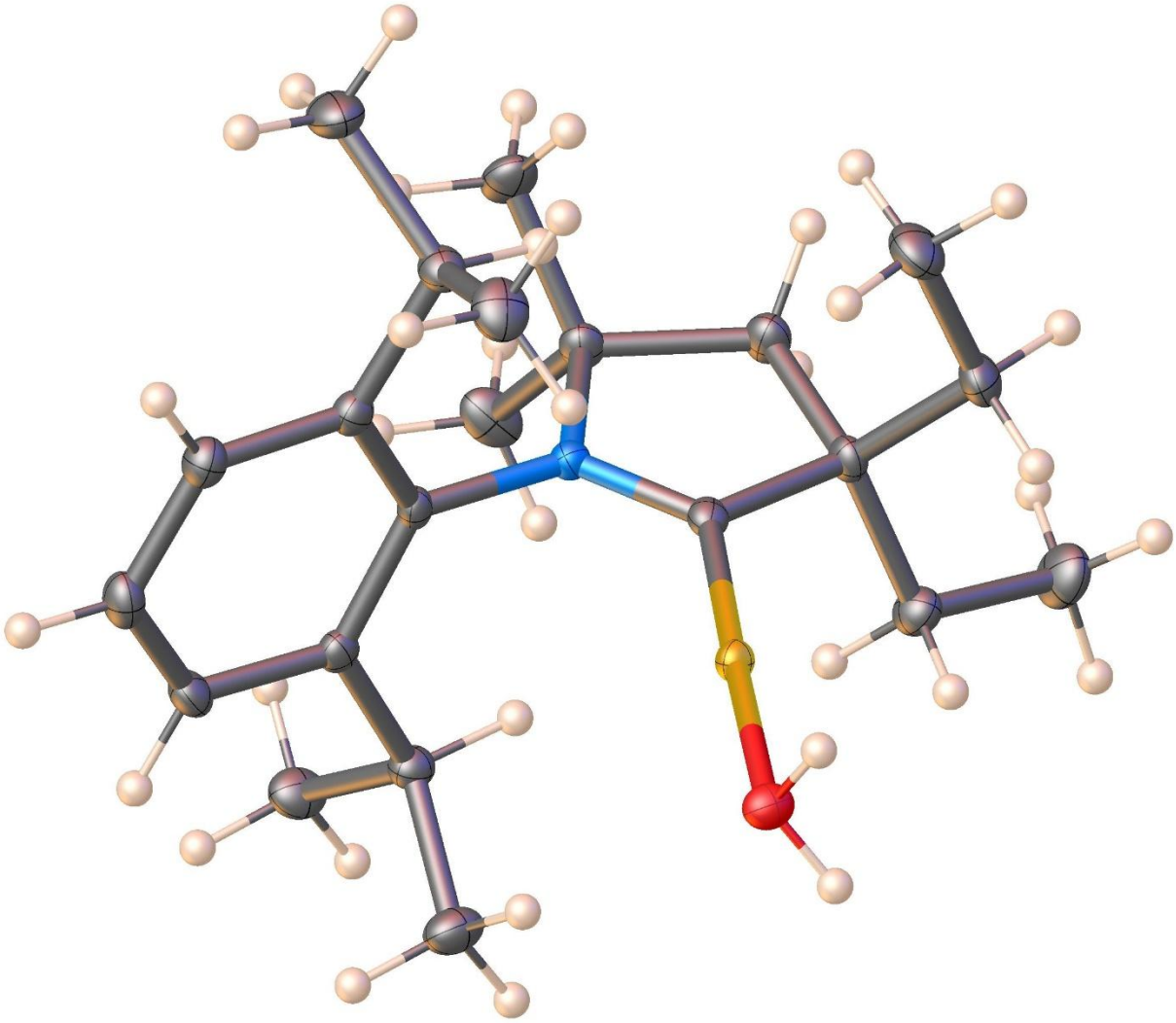

Figure S11. Molecular structures of [(^{Et2}CAAC)Au(OH_2)][SbF_6]. The [SbF_6]$^-$ counter ion has been omitted for clarity.

Table S8 Crystal data and structure refinement for [(^{Et2}CAAC)Au(OH_2)][SbF_6].

Empirical formula	$C_{22}H_{37}AuF_6NOSb$
Formula weight	764.24
Temperature/K	100.01
Crystal system	orthorhombic
Space group	Pbca
a/Å	12.9320(5)
b/Å	16.4501(6)
c/Å	24.4593(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5203.3(3)
Z	8
ρ_{calc}g/cm^3	1.951
μ/mm^{-1}	6.728
F(000)	2944.0
Crystal size/mm^3	0.16 × 0.15 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.21 to 66.65
Index ranges	$-19 \leq h \leq 19$, $-25 \leq k \leq 25$, $-37 \leq l \leq 37$
Reflections collected	81547
Independent reflections	10017 [R_{int} = 0.0461, R_{sigma} = 0.0250]
Data/restraints/parameters	10017/0/299
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0233, wR_2 = 0.0427
Final R indexes [all data]	R_1 = 0.0349, wR_2 = 0.0458
Largest diff. peak/hole / e Å^{-3}	1.17/-0.80

Table S9. Energy decomposition analysis for for $[(NHC)M]^{+}\cdots OEt_2$ interaction. Values in kcal·mol^{-1}.

	1		**2**		**3**	
ΔE^{Pauli}	65.9		48.6		73.7	
ΔE^{Elstat}	-66.6	57.7%	-50.0	58.7%	-69.7	57.3%
ΔE^{Orb}	-31.1	26.9%	-23.2	27.3%	-38.0	31.3%
ΔE^{Disp}	-17.9	15.4%	-11.9	14.0%	-13.9	11.4%
ΔE^{Int}	-49.6		-36.6		-48.0	
	4		**5**		**6**	
ΔE^{Pauli}	60.1		42.8		70.2	
ΔE^{Elstat}	-61.6	57.8%	-44.9	58.1%	-65.9	57.3%
ΔE^{Orb}	-30.2	28.3%	-21.6	27.9%	-36.6	31.8%
ΔE^{Disp}	-14.8	13.9%	-10.8	14.0%	-12.5	10.9%
ΔE^{Int}	-46.5		-34.5		-44.8	

Table S10. Energy decomposition analysis for for $[(NHC)M]^{+}\cdots OH_2$ interaction. Values in kcal·mol^{-1}.

	7		**8**		**9**	
ΔE^{Pauli}	36.3		28.2		48.4	
ΔE^{Elstat}	-44.4	66.7%	-34.8	69.3%	-50.8	64.6%
ΔE^{Orb}	-19.1	28.7%	-13.9	27.6%	-26.1	33.1%
ΔE^{Disp}	-3.1	4.6%	-1.6	3.1%	-1.8	2.3%
ΔE^{Int}	-30.2		-22.0		-30.3	
	10		**11**		**12**	
ΔE^{Pauli}	37.8		26.3		48.2	
ΔE^{Elstat}	-45.4	67.3%	-32.7	68.9%	-49.4	64.4%
ΔE^{Orb}	-19.1	28.4%	-13.2	27.8%	-25.5	33.3%
ΔE^{Disp}	-2.9	4.3%	-1.6	3.3%	-1.8	2.3%
ΔE^{Int}	-29.6		-21.1		-28.5	

Table S11. Energy decomposition analysis for $[(SIPr)I]^{+}\cdots OEt_2$ (13) and $[(SIPr)I]^{+}\cdots OH_2$ (14) interaction. Values in kcal·mol^{-1}.

	13		**14**	
ΔE^{Pauli}	19.64		11.05	
ΔE^{Elstat}	-16.03	48.5%	-12.05	66.4%
ΔE^{Orb}	-9.2	27.8%	-4.8	26.4%
ΔE^{Disp}	-7.8	23.7%	-1.3	7.3%
ΔE^{Int}	-13.4		-7.1	

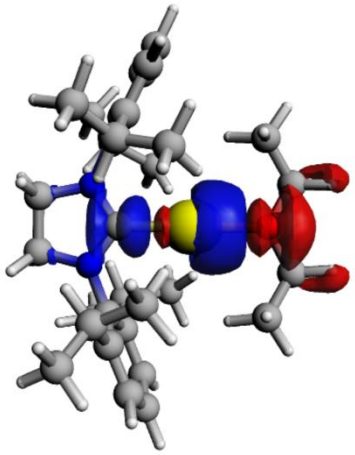

Figure S11. Relevant charge-transfer related to the $[(NHC)M]^{+}\cdots OEt_2$ interaction, as a representative case for all the studied species accounting for the ΔE^{Orb} term. Charge flow from red to blue isosurfaces.

Table S12. Energy decomposition analysis for imidazole-2-thione derivative of 1 for interaction toward, OEt_2, OH_2 and SH_2 solvent molecules. Values in kcal·mol^{-1}.

	$\cdots OEt_2$		**$\cdots OH_2$**		**$\cdots SH_2$**	
ΔE^{Pauli}	9.6		14.3		10.0	
ΔE^{Elstat}	-5.7	34.2%	-11.7	49.8%	-6.9	41.1%
ΔE^{Orb}	-3.9	23.3%	-8.5	36.2%	-5.7	33.9%
ΔE^{Disp}	-7.1	42.5%	-3.3	14.0%	-4.2	25.1%
ΔE^{Int}	-7.0		-9.2		-6.8	

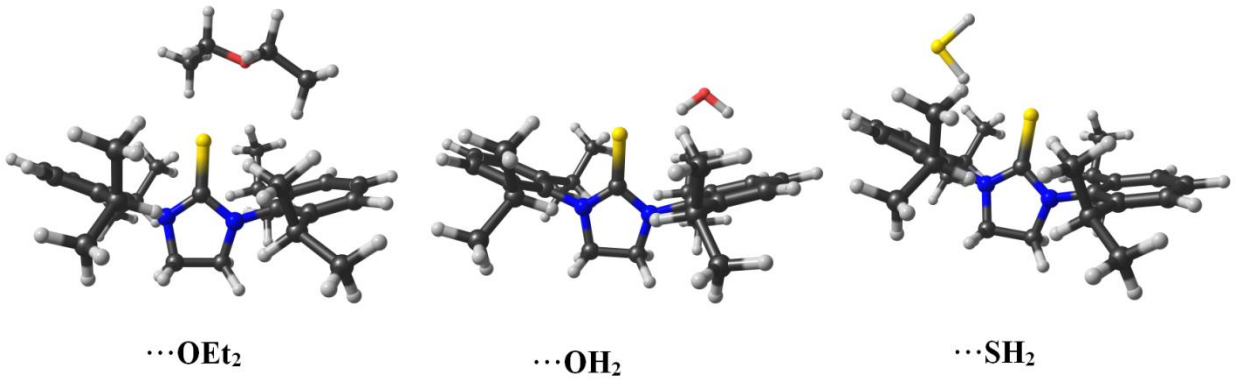

Figure S12. Optimized structures for imidazole-2-thione derivative of 1 for interaction toward, OEt_2, OH_2 and SH_2 solvent molecules, denoting the lesser interaction.

Table S13. Coordinates for optimized structures, in a multipleXYZ format. Distances in Angstrom (Å).

```
83
1
O         0.0158      0.0289      3.1849
C         1.2388     -0.3779      3.8938
H         1.1983     -1.4683      4.0490
H         1.2215      0.1247      4.8731
C        -1.2241     -0.3309      3.8866
H        -1.2481     -1.4263      4.0014
H        -1.1752      0.1339      4.8825
C        -2.4018      0.1796      3.0843
H        -2.2984      1.2540      2.8836
H        -2.5099     -0.3520      2.1265
H        -3.3275      0.0227      3.6541
C         2.4409      0.0352      3.0723
H         3.3591     -0.1843      3.6340
H         2.4963     -0.5101      2.1180
H         2.4207      1.1115      2.8558
Cu        0.0037      0.0410      1.2514
N         1.0892      0.0782     -1.3846
N        -1.0987     -0.0495     -1.3841
C        -0.0052      0.0296     -0.6110
C         0.7379      0.1958     -2.8233
H         1.3755     -0.4524     -3.4356
H         0.8806      1.2393     -3.1448
C        -0.7431     -0.2255     -2.8161
H        -1.3796      0.3960     -3.4563
H        -0.8842     -1.2816     -3.0941
```

C	2.4009	0.3345	-0.8541
C	3.2847	-0.7579	-0.7269
C	4.5478	-0.5086	-0.1784
H	5.2581	-1.3265	-0.0616
C	4.9092	0.7769	0.2293
H	5.8995	0.9528	0.6508
C	4.0127	1.8350	0.1028
H	4.3088	2.8320	0.4321
C	2.7352	1.6396	-0.4419
C	2.8328	-2.1697	-1.0758
H	2.0505	-2.0905	-1.8458
C	3.9525	-3.0543	-1.6403
H	4.4601	-2.5698	-2.4847
H	3.5374	-4.0094	-1.9892
H	4.7083	-3.2903	-0.8789
C	2.1846	-2.8206	0.1622
H	1.8078	-3.8253	-0.0754
H	1.3408	-2.2181	0.5312
H	2.9187	-2.9132	0.9752
C	1.7628	2.8067	-0.5444
H	0.8235	2.4375	-0.9816
C	2.3048	3.9130	-1.4671
H	3.2243	4.3574	-1.0606
H	1.5651	4.7180	-1.5765
H	2.5386	3.5192	-2.4656
C	1.4166	3.3585	0.8502
H	0.9731	2.5751	1.4844
H	0.6915	4.1794	0.7715
H	2.3095	3.7419	1.3632
C	-2.4109	-0.3018	-0.8525
C	-2.7389	-1.5980	-0.4068
C	-4.0237	-1.7919	0.1218
H	-4.3152	-2.7820	0.4747
C	-4.9313	-0.7390	0.2070
H	-5.9264	-0.9127	0.6181
C	-4.5733	0.5391	-0.2252
H	-5.2912	1.3539	-0.1374
C	-3.3053	0.7853	-0.7637
C	-1.7488	-2.7536	-0.4442
H	-0.8052	-2.3873	-0.8742
C	-1.4275	-3.2424	0.9806
H	-1.0215	-2.4208	1.5930
H	-0.6801	-4.0468	0.9547
H	-2.3247	-3.6260	1.4854
C	-2.2523	-3.9054	-1.3320
H	-3.1749	-4.3466	-0.9295
H	-1.4985	-4.7030	-1.3905

H	-2.4677	-3.5565	-2.3513
C	-2.8591	2.1904	-1.1447
H	-2.0804	2.0954	-1.9170
C	-2.2065	2.8667	0.0774
H	-2.9383	2.9756	0.8903
H	-1.8310	3.8662	-0.1829
H	-1.3629	2.2714	0.4575
C	-3.9833	3.0611	-1.7217
H	-4.7357	3.3115	-0.9610
H	-4.4945	2.5598	-2.5544
H	-3.5714	4.0097	-2.0912

83

2

O	0.0604	0.0764	3.5719
C	1.3444	-0.2258	4.2098
H	1.4268	-1.3192	4.3298
H	1.3287	0.2379	5.2083
C	-1.0875	-0.4402	4.3208
H	-0.9727	-1.5315	4.4285
H	-1.0589	0.0184	5.3212
C	-2.3634	-0.0836	3.5853
H	-2.4365	1.0004	3.4252
H	-2.4336	-0.5951	2.6115
H	-3.2284	-0.3995	4.1842
C	2.4691	0.3309	3.3597
H	3.4287	0.1490	3.8609
H	2.5209	-0.1541	2.3710
H	2.3593	1.4142	3.2146
Ag	-0.0162	0.0621	1.3821
N	1.0784	0.0911	-1.4370
N	-1.1060	-0.0631	-1.4617
C	-0.0240	0.0296	-0.6825
C	0.7487	0.1906	-2.8838
H	1.3916	-0.4720	-3.4749
H	0.9053	1.2277	-3.2179
C	-0.7367	-0.2215	-2.8945
H	-1.3635	0.4150	-3.5299
H	-0.8847	-1.2718	-3.1888
C	2.3852	0.3310	-0.8860
C	3.2445	-0.7755	-0.7244
C	4.4945	-0.5444	-0.1378
H	5.1845	-1.3751	0.0086
C	4.8673	0.7376	0.2690
H	5.8469	0.8993	0.7205
C	3.9959	1.8116	0.1026
H	4.3018	2.8064	0.4295
C	2.7321	1.6348	-0.4782

C	2.7893	-2.1830	-1.0854
H	1.9770	-2.0941	-1.8226
C	3.8970	-3.0396	-1.7163
H	4.3578	-2.5308	-2.5737
H	3.4817	-3.9951	-2.0642
H	4.6915	-3.2758	-0.9950
C	2.1945	-2.8683	0.1607
H	1.8344	-3.8778	-0.0824
H	1.3481	-2.2910	0.5616
H	2.9532	-2.9550	0.9515
C	1.7901	2.8207	-0.6338
H	0.8430	2.4568	-1.0585
C	2.3679	3.8663	-1.6055
H	3.2999	4.2983	-1.2147
H	1.6543	4.6883	-1.7550
H	2.5932	3.4200	-2.5838
C	1.4548	3.4517	0.7293
H	1.0103	2.7100	1.4102
H	0.7358	4.2727	0.6069
H	2.3522	3.8579	1.2161
C	-2.4251	-0.3032	-0.9417
C	-2.7642	-1.5970	-0.4973
C	-4.0465	-1.7761	0.0415
H	-4.3482	-2.7638	0.3927
C	-4.9422	-0.7129	0.1324
H	-5.9360	-0.8759	0.5514
C	-4.5762	0.5594	-0.3089
H	-5.2860	1.3815	-0.2205
C	-3.3083	0.7923	-0.8549
C	-1.7980	-2.7710	-0.5739
H	-0.8403	-2.4065	-0.9735
C	-1.5082	-3.3472	0.8233
H	-1.1053	-2.5715	1.4931
H	-0.7701	-4.1579	0.7605
H	-2.4177	-3.7524	1.2879
C	-2.3182	-3.8603	-1.5294
H	-3.2587	-4.2944	-1.1624
H	-1.5859	-4.6745	-1.6207
H	-2.5097	-3.4525	-2.5312
C	-2.8600	2.1929	-1.2501
H	-2.0364	2.0897	-1.9730
C	-2.2892	2.9202	-0.0159
H	-3.0625	3.0292	0.7576
H	-1.9292	3.9230	-0.2858
H	-1.4487	2.3606	0.4202
C	-3.9646	3.0220	-1.9210
H	-4.7704	3.2737	-1.2175

H	-4.4100	2.4854	-2.7695
H	-3.5511	3.9702	-2.2904

83

3

O	0.0227	0.1262	3.4451
C	1.2902	-0.2087	4.1285
H	1.3445	-1.3085	4.2272
H	1.2227	0.2408	5.1348
C	-1.1565	-0.4008	4.1621
H	-1.0620	-1.5007	4.2121
H	-1.1058	0.0123	5.1843
C	-2.4220	0.0295	3.4491
H	-2.4565	1.1232	3.3291
H	-2.5225	-0.4421	2.4563
H	-3.2860	-0.2784	4.0548
C	2.4602	0.3519	3.3434
H	3.3798	0.1908	3.9244
H	2.5882	-0.1469	2.3654
H	2.3457	1.4354	3.1741
Au	-0.0027	0.0437	1.3102
N	1.0898	0.0805	-1.4211
N	-1.1036	-0.0869	-1.4312
C	-0.0123	0.0086	-0.6646
C	0.7476	0.1799	-2.8611
H	1.3806	-0.4902	-3.4545
H	0.9105	1.2144	-3.1998
C	-0.7434	-0.2213	-2.8648
H	-1.3697	0.4345	-3.4810
H	-0.9033	-1.2636	-3.1799
C	2.3991	0.3243	-0.8757
C	3.2560	-0.7815	-0.7056
C	4.5071	-0.5451	-0.1233
H	5.1958	-1.3756	0.0318
C	4.8814	0.7405	0.2694
H	5.8616	0.9060	0.7182
C	4.0104	1.8139	0.0940
H	4.3170	2.8115	0.4114
C	2.7451	1.6321	-0.4808
C	2.8033	-2.1927	-1.0532
H	1.9513	-2.1108	-1.7450
C	3.8918	-3.0208	-1.7530
H	4.2901	-2.4972	-2.6323
H	3.4798	-3.9846	-2.0816
H	4.7322	-3.2401	-1.0801
C	2.2882	-2.9009	0.2156
H	1.9222	-3.9096	-0.0227
H	1.4650	-2.3353	0.6773

H	3.0945	-2.9951	0.9571
C	1.8017	2.8154	-0.6449
H	0.8498	2.4450	-1.0535
C	2.3708	3.8430	-1.6405
H	3.3073	4.2796	-1.2659
H	1.6573	4.6638	-1.7968
H	2.5865	3.3801	-2.6134
C	1.4784	3.4682	0.7104
H	1.0377	2.7356	1.4023
H	0.7593	4.2877	0.5791
H	2.3799	3.8831	1.1822
C	-2.4207	-0.3218	-0.9013
C	-2.7696	-1.6229	-0.4875
C	-4.0477	-1.7999	0.0602
H	-4.3577	-2.7926	0.3895
C	-4.9274	-0.7271	0.1926
H	-5.9179	-0.8885	0.6198
C	-4.5481	0.5525	-0.2138
H	-5.2430	1.3829	-0.0894
C	-3.2845	0.7836	-0.7708
C	-1.8124	-2.8017	-0.5929
H	-0.8562	-2.4367	-0.9963
C	-1.5108	-3.3974	0.7941
H	-1.1032	-2.6282	1.4674
H	-0.7727	-4.2066	0.7122
H	-2.4167	-3.8113	1.2582
C	-2.3489	-3.8737	-1.5588
H	-3.2881	-4.3075	-1.1878
H	-1.6230	-4.6912	-1.6688
H	-2.5486	-3.4512	-2.5532
C	-2.8264	2.1900	-1.1295
H	-1.9603	2.0992	-1.8025
C	-2.3385	2.9151	0.1406
H	-3.1615	3.0217	0.8616
H	-1.9635	3.9189	-0.1034
H	-1.5296	2.3534	0.6309
C	-3.9005	3.0078	-1.8621
H	-4.7552	3.2344	-1.2099
H	-4.2794	2.4736	-2.7434
H	-3.4825	3.9682	-2.1930

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O	-0.6485	0.2779	-1.7304
C	-1.2151	1.6077	-1.9848
H	-1.8588	1.5166	-2.8722
H	-0.3895	2.2997	-2.2143
C	-2.0067	2.0510	-0.7740

H	-2.5128	3.0020	-0.9912
H	-1.3529	2.2079	0.0968
H	-2.7683	1.3032	-0.5131
C	0.0747	-0.2534	-2.8973
H	0.9765	0.3605	-3.0486
H	-0.5896	-0.1303	-3.7648
C	0.4104	-1.7057	-2.6556
H	0.9172	-2.1113	-3.5420
H	-0.4984	-2.2931	-2.4735
H	1.0914	-1.8313	-1.7999
Cu	0.0357	-0.1459	0.0603
N	1.5808	-1.4761	1.9818
C	0.7320	-0.5028	1.7548
C	0.4636	0.2619	3.0331
C	1.5757	-0.2433	3.9933
H	2.3961	0.4884	4.0187
H	1.2139	-0.3684	5.0214
C	2.1009	-1.5781	3.4224
C	-0.9495	-0.1399	3.5624
H	-0.9646	-1.2308	3.7096
H	-1.0503	0.2993	4.5669
C	-2.1449	0.2688	2.6975
H	-2.1053	-0.2013	1.7036
H	-2.1940	1.3566	2.5537
H	-3.0840	-0.0438	3.1745
C	0.5752	1.7800	2.7584
H	1.5805	1.9757	2.3501
H	-0.1294	2.0435	1.9539
C	0.3268	2.6650	3.9826
H	0.5062	3.7206	3.7385
H	0.9937	2.3991	4.8150
H	-0.7078	2.5798	4.3424
C	3.6274	-1.6755	3.4544
H	4.1061	-0.7924	3.0149
H	3.9811	-2.5730	2.9286
H	3.9497	-1.7469	4.5024
C	1.5112	-2.8153	4.1100
H	1.8067	-3.7316	3.5824
H	0.4169	-2.7782	4.1710
H	1.9064	-2.8711	5.1336
C	1.9364	-2.4389	0.9500
C	1.0904	-3.5492	0.7369
C	1.4869	-4.4817	-0.2326
H	0.8590	-5.3538	-0.4192
C	2.6566	-4.3086	-0.9685
H	2.9519	-5.0547	-1.7062
C	3.4321	-3.1658	-0.7854

H	4.3171	-3.0125	-1.4037
C	3.0848	-2.1980	0.1669
C	-0.2623	-3.7107	1.4223
H	-0.3446	-2.9436	2.2002
C	-1.3983	-3.4433	0.4158
H	-1.3728	-4.1680	-0.4110
H	-1.3140	-2.4343	-0.0185
H	-2.3770	-3.5230	0.9107
C	-0.4406	-5.0832	2.0908
H	0.3690	-5.3006	2.7998
H	-0.4609	-5.8931	1.3482
H	-1.3934	-5.1165	2.6380
C	3.8651	-0.8902	0.2313
H	3.5262	-0.3348	1.1142
C	3.5261	-0.0192	-0.9944
H	2.4491	0.2161	-1.0207
H	3.7834	-0.5374	-1.9297
H	4.0813	0.9292	-0.9613
C	5.3822	-1.1021	0.3531
H	5.7989	-1.5599	-0.5549
H	5.6315	-1.7532	1.2010
H	5.8907	-0.1385	0.4963

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O	-0.7513	0.3183	-2.0885
C	-1.2623	1.6515	-2.4038
H	-1.8410	1.5696	-3.3372
H	-0.4091	2.3292	-2.5794
C	-2.1351	2.1309	-1.2649
H	-2.5817	3.1022	-1.5224
H	-1.5521	2.2657	-0.3402
H	-2.9489	1.4176	-1.0720
C	0.0560	-0.2381	-3.1748
H	0.9630	0.3786	-3.2906
H	-0.5422	-0.1600	-4.0963
C	0.3930	-1.6800	-2.8618
H	0.9402	-2.1178	-3.7078
H	-0.5197	-2.2695	-2.6983
H	1.0405	-1.7703	-1.9745
Ag	-0.0493	-0.1184	-0.0107
N	1.5831	-1.4812	2.0591
C	0.7249	-0.5128	1.8775
C	0.4826	0.2279	3.1720
C	1.6215	-0.2882	4.0949
H	2.4366	0.4488	4.1168
H	1.2842	-0.4358	5.1281
C	2.1393	-1.6077	3.4885

C	-0.9127	-0.1943	3.7365
H	-0.9273	-1.2910	3.8353
H	-0.9652	0.1977	4.7644
C	-2.1447	0.2613	2.9516
H	-2.1637	-0.1628	1.9369
H	-2.1928	1.3558	2.8608
H	-3.0599	-0.0659	3.4650
C	0.5771	1.7538	2.9340
H	1.5680	1.9679	2.4996
H	-0.1575	2.0402	2.1656
C	0.3690	2.5972	4.1953
H	0.5360	3.6611	3.9781
H	1.0652	2.3116	4.9963
H	-0.6523	2.4967	4.5876
C	3.6645	-1.6957	3.4781
H	4.1246	-0.8047	3.0357
H	4.0106	-2.5848	2.9341
H	4.0150	-1.7754	4.5161
C	1.5702	-2.8574	4.1673
H	1.8595	-3.7643	3.6202
H	0.4777	-2.8278	4.2528
H	1.9877	-2.9269	5.1812
C	1.9287	-2.4192	0.9970
C	1.0933	-3.5380	0.7830
C	1.4673	-4.4347	-0.2284
H	0.8461	-5.3104	-0.4176
C	2.6037	-4.2212	-1.0038
H	2.8781	-4.9372	-1.7779
C	3.3716	-3.0754	-0.8104
H	4.2310	-2.8897	-1.4547
C	3.0480	-2.1408	0.1832
C	-0.2306	-3.7526	1.5101
H	-0.3210	-2.9901	2.2919
C	-1.4093	-3.5398	0.5416
H	-1.3900	-4.2783	-0.2729
H	-1.3765	-2.5378	0.0864
H	-2.3665	-3.6444	1.0730
C	-0.3298	-5.1331	2.1799
H	0.5059	-5.3189	2.8663
H	-0.3335	-5.9404	1.4343
H	-1.2657	-5.2102	2.7512
C	3.8315	-0.8345	0.2583
H	3.4787	-0.2728	1.1326
C	3.5325	0.0334	-0.9801
H	2.4565	0.2578	-1.0558
H	3.8357	-0.4789	-1.9044
H	4.0767	0.9870	-0.9244

C	5.3455	-1.0560	0.4084
H	5.7705	-1.5292	-0.4881
H	5.5822	-1.6976	1.2670
H	5.8588	-0.0935	0.5453

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O	-0.7659	0.2781	-1.9387
C	-1.3228	1.6154	-2.2046
H	-1.8360	1.5490	-3.1755
H	-0.4879	2.3280	-2.2907
C	-2.2854	1.9921	-1.1019
H	-2.7640	2.9492	-1.3523
H	-1.7689	2.1113	-0.1377
H	-3.0689	1.2307	-0.9923
C	0.0665	-0.2099	-3.0555
H	0.9629	0.4268	-3.1196
H	-0.5341	-0.0749	-3.9670
C	0.4148	-1.6639	-2.8354
H	0.9516	-2.0382	-3.7181
H	-0.4926	-2.2666	-2.6996
H	1.0694	-1.8041	-1.9617
Au	0.0032	-0.1105	0.0441
N	1.5938	-1.4797	2.0273
C	0.7520	-0.4945	1.8326
C	0.4899	0.2651	3.1147
C	1.6135	-0.2604	4.0503
H	2.4392	0.4652	4.0703
H	1.2651	-0.3922	5.0820
C	2.1209	-1.5945	3.4627
C	-0.9163	-0.1374	3.6680
H	-0.9469	-1.2337	3.7684
H	-0.9664	0.2579	4.6947
C	-2.1392	0.3359	2.8779
H	-2.1644	-0.0932	1.8655
H	-2.1655	1.4306	2.7795
H	-3.0596	0.0295	3.3945
C	0.6064	1.7888	2.8674
H	1.6031	1.9868	2.4395
H	-0.1171	2.0792	2.0903
C	0.3989	2.6414	4.1220
H	0.5786	3.7013	3.8977
H	1.0868	2.3532	4.9295
H	-0.6263	2.5549	4.5078
C	3.6454	-1.7024	3.4775
H	4.1235	-0.8225	3.0318
H	3.9867	-2.6029	2.9488
H	3.9774	-1.7752	4.5225

C	1.5257	-2.8306	4.1444
H	1.8156	-3.7453	3.6114
H	0.4321	-2.7883	4.2085
H	1.9245	-2.8925	5.1664
C	1.9457	-2.4302	0.9771
C	1.1072	-3.5468	0.7632
C	1.4993	-4.4629	-0.2237
H	0.8772	-5.3390	-0.4103
C	2.6510	-4.2656	-0.9812
H	2.9374	-4.9957	-1.7379
C	3.4181	-3.1182	-0.7935
H	4.2888	-2.9452	-1.4266
C	3.0811	-2.1680	0.1805
C	-0.2368	-3.7394	1.4582
H	-0.3416	-2.9628	2.2249
C	-1.3862	-3.5317	0.4525
H	-1.3472	-4.2813	-0.3511
H	-1.3310	-2.5352	-0.0113
H	-2.3583	-3.6247	0.9575
C	-0.3669	-5.1082	2.1467
H	0.4517	-5.2938	2.8539
H	-0.3652	-5.9259	1.4128
H	-1.3161	-5.1649	2.6981
C	3.8687	-0.8644	0.2527
H	3.5035	-0.2911	1.1145
C	3.5909	-0.0103	-0.9998
H	2.5161	0.2145	-1.0877
H	3.9061	-0.5356	-1.9132
H	4.1387	0.9415	-0.9466
C	5.3795	-1.0901	0.4302
H	5.8179	-1.5698	-0.4563
H	5.5987	-1.7279	1.2960
H	5.8936	-0.1287	0.5703

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O	0.0303	-0.0364	3.2289
H	-0.3847	0.6236	3.8155
H	0.3908	-0.7485	3.7879
Cu	0.0083	-0.0155	1.2509
N	1.0886	0.0676	-1.3895
N	-1.1005	-0.0438	-1.3909
C	-0.0063	0.0055	-0.6182
C	0.7383	0.2195	-2.8254
H	1.3670	-0.4280	-3.4477
H	0.9030	1.2662	-3.1248
C	-0.7483	-0.1739	-2.8289
H	-1.3766	0.4827	-3.4418

H	-0.9130	-1.2160	-3.1436
C	2.4133	0.3144	-0.8885
C	3.3033	-0.7776	-0.8163
C	4.5947	-0.5267	-0.3388
H	5.3132	-1.3426	-0.2655
C	4.9763	0.7595	0.0490
H	5.9886	0.9362	0.4144
C	4.0730	1.8174	-0.0240
H	4.3863	2.8141	0.2898
C	2.7671	1.6203	-0.4963
C	2.8338	-2.1856	-1.1582
H	2.0331	-2.0990	-1.9094
C	3.9331	-3.0761	-1.7542
H	4.4205	-2.5930	-2.6119
H	3.5030	-4.0279	-2.0934
H	4.7082	-3.3180	-1.0135
C	2.2101	-2.8385	0.0922
H	1.8327	-3.8447	-0.1383
H	1.3685	-2.2389	0.4730
H	2.9580	-2.9252	0.8932
C	1.7832	2.7813	-0.5391
H	0.8342	2.4169	-0.9592
C	2.2823	3.9235	-1.4404
H	3.2064	4.3695	-1.0474
H	1.5280	4.7204	-1.5024
H	2.4919	3.5658	-2.4575
C	1.4761	3.2838	0.8828
H	1.0921	2.4639	1.5116
H	0.7201	4.0803	0.8588
H	2.3774	3.6797	1.3702
C	-2.4280	-0.2935	-0.8997
C	-2.7882	-1.6029	-0.5259
C	-4.0986	-1.8020	-0.0671
H	-4.4171	-2.8016	0.2322
C	-5.0003	-0.7431	0.0091
H	-6.0165	-0.9216	0.3626
C	-4.6125	0.5465	-0.3611
H	-5.3302	1.3630	-0.2862
C	-3.3163	0.7997	-0.8234
C	-1.8074	-2.7660	-0.5758
H	-0.8558	-2.3999	-0.9886
C	-1.5074	-3.2828	0.8428
H	-1.1261	-2.4692	1.4813
H	-0.7522	-4.0799	0.8146
H	-2.4117	-3.6827	1.3219
C	-2.3057	-3.8987	-1.4896
H	-3.2320	-4.3467	-1.1040

H	-1.5529	-4.6966	-1.5563
H	-2.5109	-3.5309	-2.5039
C	-2.8391	2.2099	-1.1449
H	-2.0393	2.1300	-1.8978
C	-2.2106	2.8396	0.1151
H	-2.9590	2.9227	0.9160
H	-1.8236	3.8452	-0.1015
H	-1.3758	2.2267	0.4891
C	-3.9328	3.1161	-1.7269
H	-4.7056	3.3526	-0.9822
H	-4.4240	2.6492	-2.5913
H	-3.4965	4.0698	-2.0527

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O	0.0050	-0.0810	3.7252
H	-0.7325	0.3697	4.1827
H	0.0536	-0.9674	4.1332
Ag	-0.0167	-0.0239	1.4728
N	1.0949	0.0796	-1.3764
N	-1.0911	-0.0543	-1.3729
C	0.0041	0.0086	-0.6067
C	0.7399	0.2225	-2.8149
H	1.3721	-0.4245	-3.4339
H	0.8990	1.2686	-3.1181
C	-0.7442	-0.1799	-2.8143
H	-1.3790	0.4744	-3.4229
H	-0.9042	-1.2223	-3.1300
C	2.4217	0.3279	-0.8819
C	3.3091	-0.7653	-0.8028
C	4.5967	-0.5151	-0.3148
H	5.3130	-1.3321	-0.2331
C	4.9777	0.7715	0.0713
H	5.9868	0.9471	0.4459
C	4.0799	1.8326	-0.0202
H	4.3957	2.8314	0.2842
C	2.7774	1.6369	-0.5017
C	2.8505	-2.1726	-1.1635
H	2.0336	-2.0808	-1.8961
C	3.9515	-3.0293	-1.8055
H	4.4129	-2.5157	-2.6597
H	3.5295	-3.9791	-2.1607
H	4.7459	-3.2772	-1.0880
C	2.2628	-2.8680	0.0810
H	1.9088	-3.8785	-0.1674
H	1.4128	-2.2995	0.4869
H	3.0242	-2.9534	0.8692
C	1.8098	2.8089	-0.5950

H	0.8471	2.4353	-0.9743
C	2.3162	3.8753	-1.5835
H	3.2579	4.3233	-1.2372
H	1.5794	4.6840	-1.6878
H	2.4998	3.4435	-2.5769
C	1.5363	3.4186	0.7908
H	1.1547	2.6578	1.4891
H	0.7901	4.2214	0.7181
H	2.4497	3.8428	1.2301
C	-2.4151	-0.2954	-0.8690
C	-2.7765	-1.6023	-0.4853
C	-4.0727	-1.7881	0.0166
H	-4.3926	-2.7851	0.3230
C	-4.9607	-0.7199	0.1232
H	-5.9655	-0.8879	0.5123
C	-4.5755	0.5637	-0.2687
H	-5.2842	1.3862	-0.1768
C	-3.2934	0.8044	-0.7759
C	-1.8208	-2.7826	-0.5976
H	-0.8610	-2.4160	-0.9901
C	-1.5310	-3.4022	0.7807
H	-1.1244	-2.6473	1.4723
H	-0.7960	-4.2136	0.6924
H	-2.4418	-3.8153	1.2355
C	-2.3526	-3.8409	-1.5815
H	-3.2930	-4.2812	-1.2221
H	-1.6251	-4.6558	-1.7004
H	-2.5474	-3.4032	-2.5701
C	-2.8304	2.2088	-1.1426
H	-2.0204	2.1118	-1.8818
C	-2.2278	2.9038	0.0948
H	-2.9823	2.9987	0.8886
H	-1.8690	3.9108	-0.1604
H	-1.3778	2.3322	0.4958
C	-3.9328	3.0692	-1.7771
H	-4.7201	3.3224	-1.0535
H	-4.4038	2.5563	-2.6265
H	-3.5093	4.0163	-2.1375

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O	-0.0633	-0.0057	3.5726
H	-0.0013	0.9044	3.9301
H	0.7166	-0.4780	3.9330
Au	-0.0403	0.0037	1.3877
N	1.0832	0.0849	-1.3450
N	-1.1126	-0.0554	-1.3657
C	-0.0221	0.0092	-0.5941

C	0.7426	0.2195	-2.7840
H	1.3773	-0.4377	-3.3897
H	0.9127	1.2616	-3.0942
C	-0.7460	-0.1738	-2.7998
H	-1.3695	0.4903	-3.4094
H	-0.9105	-1.2125	-3.1240
C	2.4070	0.3186	-0.8341
C	3.2772	-0.7860	-0.7398
C	4.5605	-0.5507	-0.2327
H	5.2641	-1.3775	-0.1375
C	4.9524	0.7322	0.1543
H	5.9583	0.8964	0.5425
C	4.0699	1.8052	0.0450
H	4.3951	2.8013	0.3488
C	2.7724	1.6249	-0.4544
C	2.8100	-2.1889	-1.1045
H	1.9595	-2.0896	-1.7966
C	3.8877	-3.0213	-1.8151
H	4.2995	-2.4881	-2.6823
H	3.4605	-3.9710	-2.1643
H	4.7204	-3.2695	-1.1427
C	2.2843	-2.9113	0.1518
H	1.9122	-3.9136	-0.1028
H	1.4619	-2.3480	0.6179
H	3.0865	-3.0211	0.8953
C	1.8197	2.8073	-0.5659
H	0.8573	2.4427	-0.9551
C	2.3516	3.8622	-1.5534
H	3.2936	4.3011	-1.1965
H	1.6257	4.6785	-1.6723
H	2.5441	3.4226	-2.5419
C	1.5335	3.4271	0.8131
H	1.1219	2.6704	1.4986
H	0.8033	4.2428	0.7246
H	2.4469	3.8353	1.2671
C	-2.4429	-0.3106	-0.8798
C	-2.7998	-1.6272	-0.5293
C	-4.1035	-1.8293	-0.0554
H	-4.4224	-2.8333	0.2273
C	-4.9981	-0.7672	0.0591
H	-6.0077	-0.9480	0.4296
C	-4.6133	0.5266	-0.2970
H	-5.3263	1.3443	-0.1958
C	-3.3248	0.7840	-0.7788
C	-1.8330	-2.7979	-0.6438
H	-0.8646	-2.4158	-1.0005
C	-1.5751	-3.4479	0.7267

H	-1.1971	-2.7073	1.4473
H	-0.8311	-4.2509	0.6358
H	-2.4937	-3.8829	1.1436
C	-2.3306	-3.8332	-1.6692
H	-3.2774	-4.2873	-1.3458
H	-1.5955	-4.6412	-1.7883
H	-2.5026	-3.3729	-2.6521
C	-2.8635	2.1978	-1.1074
H	-2.0156	2.1197	-1.8058
C	-2.3361	2.8887	0.1661
H	-3.1349	2.9710	0.9166
H	-1.9719	3.9003	-0.0623
H	-1.5084	2.3180	0.6133
C	-3.9458	3.0477	-1.7898
H	-4.7743	3.2775	-1.1057
H	-4.3626	2.5375	-2.6685
H	-3.5212	4.0066	-2.1160

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10

O	-0.5922	0.8323	1.6618
H	-0.1295	0.6645	2.5095
H	-0.7576	1.7952	1.6249
Cu	-0.0005	-0.1267	0.0115
N	1.7646	-1.4251	-1.7142
C	0.5408	-1.0037	-1.5352
C	2.0241	-2.1161	-3.0611
C	0.5839	-2.2101	-3.6183
H	0.2367	-3.2505	-3.5689
H	0.5569	-1.9079	-4.6728
C	-0.3165	-1.3002	-2.7383
C	2.8131	-1.2049	-0.7258
C	3.5332	0.0097	-0.7490
C	4.5677	0.1585	0.1867
H	5.1472	1.0825	0.1958
C	4.8550	-0.8396	1.1156
H	5.6720	-0.7050	1.8251
C	4.0764	-1.9944	1.1605
H	4.2741	-2.7471	1.9249
C	3.0304	-2.2006	0.2504
C	3.1545	1.1904	-1.6384
H	2.3804	0.8585	-2.3407
C	2.5267	2.3096	-0.7813
H	3.2514	2.7032	-0.0535
H	1.6576	1.9304	-0.2169
H	2.1887	3.1413	-1.4172
C	4.3355	1.7400	-2.4558
H	5.1129	2.1585	-1.8006

H	3.9930	2.5480	-3.1184
H	4.8012	0.9617	-3.0742
C	2.1029	-3.3981	0.4229
H	1.4473	-3.4532	-0.4537
C	1.1874	-3.1771	1.6436
H	1.7759	-3.0951	2.5690
H	0.4811	-4.0121	1.7545
H	0.6021	-2.2482	1.5315
C	2.8539	-4.7339	0.5382
H	3.5290	-4.8903	-0.3133
H	2.1395	-5.5682	0.5715
H	3.4541	-4.7802	1.4575
C	2.9436	-1.2366	-3.9149
H	2.4946	-0.2583	-4.1282
H	3.1274	-1.7438	-4.8718
H	3.9110	-1.0855	-3.4176
C	2.6736	-3.4850	-2.8537
H	3.6353	-3.3935	-2.3305
H	2.8615	-3.9347	-3.8383
H	2.0226	-4.1639	-2.2894
C	-0.6118	0.0776	-3.4066
H	-1.0279	0.7478	-2.6346
H	0.3470	0.5239	-3.7158
C	-1.5654	0.0162	-4.6047
H	-1.2162	-0.6938	-5.3684
H	-1.6399	1.0041	-5.0790
H	-2.5774	-0.2837	-4.3022
C	-1.6332	-1.9837	-2.2927
H	-2.2489	-1.2251	-1.7791
H	-2.1880	-2.2816	-3.1944
C	-1.4433	-3.1941	-1.3703
H	-0.8263	-3.9761	-1.8374
H	-2.4112	-3.6471	-1.1184
H	-0.9537	-2.9009	-0.4285

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11

O	-0.6958	1.1386	2.0427
H	-0.3922	0.8626	2.9279
H	-0.7468	2.1131	2.0626
Ag	-0.0739	0.0369	0.1585
N	1.7442	-1.4124	-1.7163
C	0.5206	-0.9952	-1.5516
C	2.0187	-2.1084	-3.0661
C	0.5856	-2.2091	-3.6322
H	0.2451	-3.2515	-3.5927
H	0.5633	-1.9016	-4.6847
C	-0.3295	-1.3094	-2.7557

C	2.7953	-1.1991	-0.7277
C	3.5259	0.0097	-0.7497
C	4.5618	0.1481	0.1856
H	5.1501	1.0664	0.1931
C	4.8407	-0.8525	1.1136
H	5.6565	-0.7231	1.8244
C	4.0571	-2.0039	1.1529
H	4.2520	-2.7608	1.9134
C	3.0111	-2.2030	0.2412
C	3.1779	1.1911	-1.6499
H	2.3950	0.8727	-2.3485
C	2.5878	2.3427	-0.8120
H	3.3181	2.7158	-0.0799
H	1.6958	2.0087	-0.2558
H	2.2942	3.1797	-1.4616
C	4.3764	1.6961	-2.4713
H	5.1515	2.1250	-1.8217
H	4.0546	2.4856	-3.1639
H	4.8401	0.8938	-3.0577
C	2.0974	-3.4136	0.4015
H	1.4231	-3.4523	-0.4621
C	1.2089	-3.2442	1.6488
H	1.8171	-3.1960	2.5636
H	0.5132	-4.0904	1.7429
H	0.6146	-2.3182	1.5884
C	2.8668	-4.7437	0.4625
H	3.5244	-4.8733	-0.4066
H	2.1629	-5.5872	0.4923
H	3.4902	-4.8051	1.3656
C	2.9409	-1.2278	-3.9137
H	2.4924	-0.2513	-4.1355
H	3.1325	-1.7387	-4.8671
H	3.9047	-1.0738	-3.4116
C	2.6729	-3.4742	-2.8600
H	3.6353	-3.3814	-2.3390
H	2.8616	-3.9195	-3.8464
H	2.0256	-4.1583	-2.2985
C	-0.6444	0.0575	-3.4384
H	-1.1094	0.7190	-2.6890
H	0.3103	0.5315	-3.7176
C	-1.5549	-0.0350	-4.6677
H	-1.1553	-0.7253	-5.4245
H	-1.6491	0.9527	-5.1389
H	-2.5652	-0.3722	-4.4030
C	-1.6358	-2.0197	-2.3201
H	-2.2691	-1.2816	-1.7995
H	-2.1813	-2.3104	-3.2293

C	-1.4313	-3.2453	-1.4216
H	-0.8094	-4.0119	-1.9064
H	-2.3960	-3.7136	-1.1824
H	-0.9465	-2.9755	-0.4722

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12

O	-0.7043	0.8775	1.9742
H	0.0668	0.9936	2.5664
H	-1.0497	1.7818	1.8229
Au	-0.0711	-0.0955	0.1038
N	1.7533	-1.4142	-1.7090
C	0.5238	-1.0074	-1.5456
C	2.0157	-2.1020	-3.0579
C	0.5838	-2.1780	-3.6372
H	0.2361	-3.2184	-3.6299
H	0.5736	-1.8396	-4.6802
C	-0.3365	-1.2959	-2.7493
C	2.8014	-1.1948	-0.7143
C	3.5283	0.0165	-0.7427
C	4.5546	0.1670	0.2013
H	5.1406	1.0867	0.2056
C	4.8260	-0.8227	1.1428
H	5.6339	-0.6844	1.8609
C	4.0454	-1.9759	1.1860
H	4.2345	-2.7237	1.9566
C	3.0079	-2.1882	0.2676
C	3.1841	1.1909	-1.6530
H	2.4023	0.8678	-2.3510
C	2.5925	2.3494	-0.8260
H	3.3243	2.7322	-0.1002
H	1.7015	2.0179	-0.2698
H	2.2989	3.1792	-1.4847
C	4.3862	1.6859	-2.4752
H	5.1633	2.1130	-1.8258
H	4.0694	2.4754	-3.1711
H	4.8470	0.8789	-3.0588
C	2.0956	-3.3980	0.4378
H	1.4082	-3.4333	-0.4161
C	1.2264	-3.2351	1.6994
H	1.8481	-3.1885	2.6051
H	0.5358	-4.0844	1.8013
H	0.6280	-2.3114	1.6506
C	2.8668	-4.7279	0.4830
H	3.5113	-4.8572	-0.3959
H	2.1632	-5.5713	0.5228
H	3.5034	-4.7899	1.3767
C	2.9575	-1.2396	-3.9019

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H        2.5267     -0.2560     -4.1273
H        3.1439     -1.7562     -4.8532
H        3.9217     -1.1011     -3.3961
C        2.6396     -3.4805     -2.8425
H        3.6031     -3.4042     -2.3210
H        2.8187     -3.9372     -3.8255
H        1.9766     -4.1443     -2.2750
C       -0.6491      0.0840     -3.4094
H       -1.1039      0.7360     -2.6463
H        0.3069      0.5560     -3.6889
C       -1.5691      0.0102     -4.6322
H       -1.1824     -0.6765     -5.3990
H       -1.6577      1.0033     -5.0931
H       -2.5803     -0.3202     -4.3613
C       -1.6432     -2.0165     -2.3314
H       -2.2865     -1.2863     -1.8128
H       -2.1720     -2.3018     -3.2527
C       -1.4448     -3.2495     -1.4420
H       -0.7920     -3.9982     -1.9150
H       -2.4071     -3.7383     -1.2405
H       -0.9985     -2.9811     -0.4727
13
81
C        2.32937598    1.11732996    3.59020209
H        2.63251209    0.59090197    4.50601101
C        1.81685901   -1.96092403    7.31190014
H        2.21527195   -1.18942797    6.63766909
C        0.47374901   -2.42871809    6.72429514
H        0.04058500   -3.24301195    7.32237816
H        0.61784500   -2.80648804    5.70302010
H       -0.25296500   -1.60558403    6.69116402
C        2.24962401    2.02638888   10.51566792
H        2.75185108    2.42323303    9.62252331
C        1.00346100    0.48892501    3.12382293
H        0.21588500    0.61925602    3.87754893
H        1.13479900   -0.58635199    2.94116092
H        0.65707898    0.94810200    2.18801594
C        2.30897689    4.96570683    6.98723793
H        2.60453892    4.12184000    7.62674093
C        3.44448304    0.90547299    2.55099010
H        3.18691111    1.37567496    1.59267104
H        3.59501600   -0.16685399    2.36659694
H        4.39665794    1.33461106    2.88888407
C        1.00492299    2.89971399   10.75997829
H        0.31263700    2.85525894    9.90853405
H        1.30010200    3.94741011   10.91145420
H        0.46333799    2.56810093   11.65657330
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C	0.98558497	5.51786995	7.54687881
H	0.65451199	6.39841986	6.97934914
H	1.11376405	5.82145977	8.59458637
H	0.18892500	4.76381493	7.50103092
C	3.24660206	2.13797808	11.68227863
H	2.79393196	1.80691898	12.62640095
H	3.56047106	3.18207502	11.81404114
H	4.14158392	1.52646005	11.50676060
C	2.83926892	-3.11206794	7.35095978
H	3.80990601	-2.77482200	7.73944378
H	2.99281907	-3.52121496	6.34294605
H	2.48523092	-3.92880106	7.99543619
C	3.43019104	6.01668596	7.06997013
H	4.38329887	5.62038898	6.69537210
H	3.57412195	6.33798790	8.11054707
H	3.18053007	6.90703106	6.47642183
I	-0.24693599	1.64339304	6.96883392
C	1.84160602	1.53180206	7.06782484
C	2.01743388	-0.02679100	8.98866367
N	2.70916295	2.18646789	6.26555777
C	2.32869506	3.10668492	5.21524620
N	2.57102990	0.78052902	7.92212486
C	4.00611591	1.84217000	6.61602783
H	4.85606289	2.25651503	6.09213495
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C	3.91992903	0.96199101	7.65297794
H	4.67910385	0.45045501	8.22776318
C	2.13374710	4.45312977	5.56511784
C	2.14855289	2.59157896	3.92100692
C	1.63828504	-1.34547400	8.69196796
C	1.07673800	-2.08527088	9.73999500
H	0.76953000	-3.11546206	9.56121063
C	1.75187194	5.31877279	4.53279495
H	1.59222305	6.37374783	4.75354719
C	1.76680303	3.50516391	2.93060088
H	1.61661899	3.15444112	1.90991294
C	0.90122002	-1.52303803	11.00274277
H	0.45937899	-2.11701798	11.80163574
C	1.57184100	4.85118580	3.23229790
H	1.27317798	5.54214096	2.44512105
O	-3.01760006	1.79882896	6.79268503
C	-3.92521501	1.05576706	7.63269806
H	-4.56981516	0.42782700	6.99286795
H	-4.57588387	1.76811898	8.16974258
C	-3.72018909	2.61781812	5.83435202

H	-4.35668612	1.96761298	5.20873785
H	-4.38285923	3.31323910	6.37923717
C	-2.72822499	3.38073897	4.97837210
H	-2.09672594	4.03762913	5.59087420
H	-2.07927203	2.69581389	4.41719723
H	-3.27143502	4.00498581	4.25649118
C	-3.14125299	0.20248400	8.60978127
H	-3.83663511	-0.35772100	9.24813175
H	-2.50366092	-0.51974702	8.08317471
H	-2.50714302	0.82201499	9.25674725