Supporting Information for

N-Heterocyclic Carbene or Phosphorus Ylide, Which one Forms a Stronger Bond with Group 11 Metals? A Theoretical Study

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Table S1. The calculated M–C bond lengths (Å) of [NHC(R) → MR′] and [{$P(Ph)_3CHR$}←MCl] (M = Cu(I), Ag(I), Au(I), R=F, Cl, Br ,CF_3, H, CH_3, $C(CH_3)_3$, $Si(CH_3)_3$, SiH_3, Ph, R′=Cl, OAc) at the PBE/def2-TZVP level of ~~theory~~.

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Bond Length		[NHC(R) → MCl]		[NHC(R) → MOAC]		[{P(Ph)3CHR}→MCl]	
R	**M**	**M-C**	**M-Cl**	**M-C**	**M-O**	**M-C**	**M-Cl**
	Cu	1.86	2.09	1.85	1.89	1.92	2.12
Br	Au	1.97	2.26	1.96	2.03	2.04	2.29
	Ag	2.04	2.28	2.04	2.11	2.11	2.31
	Cu	1.86	2.09	1.84	2.07	1.96	2.11
CF3	Au	1.98	2.26	1.96	2.02	2.09	2.29
	Ag	2.06	2.28	2.04	2.25	2.15	2.31
	Cu	1.86	2.09	1.85	1.89	1.92	2.12
Cl	Au	1.97	2.26	1.95	2.03	2.05	2.29
	Ag	2.04	2.28	2.03	2.11	2.12	2.3
	Cu	1.86	2.09	1.89	2.09	1.92	2.12
F	Au	1.97	2.26	1.95	2.03	2.04	2.3
	Ag	2.04	2.28	2.03	2.13	2.11	2.31
	Cu	1.87	2.1	1.86	1.89	1.96	2.12
Me	Au	1.99	2.27	1.97	2.04	2.09	2.3
	Ag	2.05	2.28	2.04	2.1	2.15	2.31
	Cu	1.87	2.1	1.86	1.88	1.96	2.12
Ph	Au	1.98	2.28	1.97	2.04	2.08	2.3
	Ag	2.05	2.29	2.04	2.09	2.16	2.31
	Cu	1.87	2.12	1.87	1.88	1.96	2.12
Si(CH3)3	Au	1.99	2.29	1.97	2.05	2.1	2.3

	Ag	2.06	2.3	2.05	2.1	2.17	2.32
	Cu	1.87	2.1	1.86	1.87	1.96	2.11
SiH3	Au	1.98	2.27	1.97	2.04	2.09	2.29
	Ag	2.05	2.29	2.04	2.09	2.16	2.3
	Cu	1.86	2.1	1.86	1.89	1.94	1.94
H	Au	1.97	2.27	1.96	2.03	2.07	2.3
	Ag	2.04	2.28	2.03	2.1	2.13	2.31
	Cu	1.89	2.11	1.88	1.87	1.96	2.12
C(CH3)3	Au	2.01	2.28	2	2.05	2.1	2.3
	Ag	2.09	2.09	2.08	2.1	2.17	2.31

Table S2. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [NHC(R)→ AgCl] complexes.

BSSE of [NHC(R)→ AgCl]		
R	E(HF)	E(Kcal.mol-1)
Br	0.002055	1.38
CF3	0.002196	1.49
Cl	0.002065	1.40
F	0.001992	1.35
CH_3	0.002257	1.53
Ph	0.002289	1.55
Si(CH3)3	0.002482	1.68
SiH3	0.002240	1.52
H	0.002154	1.35
C(CH3)3	0.002262	1.42

Table S3. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [NHC(R)→ AgOAc] complexes.

BSSE of [NHC(R)→ AgOAc]		
R	E(HF)	E(Kcal.mol-1)
Br	0.0017809	1.12
CF3	0.0016277	1.02
Cl	0.0018405	1.15
F	0.0016589	1.04
CH_3	0.0020759	1.30
Ph	0.0022307	1.40
Si(CH3)3	0.0025982	1.63
SiH3	0.0020903	1.31
H	0.0019555	1.23
C(CH3)3	0.0021532	1.35

Table S4. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [NHC(R)→ AuCl] complexes.

BSSE of [NHC(R)→ AuCl]		
R	E(HF)	E(Kcal.mol-1)
Br	0.001720	1.16
CF3	0.001808	1.22
Cl	0.001735	1.17
F	0.001696	1.14
CH_3	0.001849	1.24
Ph	0.001883	1.27
Si(CH3)3	0.001926	1.30
SiH3	0.001821	1.22
H	0.001846	1.24
C(CH3)3	0.001872	1.26

Table S5. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [NHC(R)→ AuOAc] complexes.

BSSE of [NHC(R)→ AuOAc]		
R	E(HF)	E(Kcal.mol-1)
Br	0.0014957	1.01
CF3	0.0017423	1.17
Cl	0.0015038	1.01
F	0.0014457	0.97
CH_3	0.0017176	1.16
Ph	0.0016163	1.09
Si(CH3)3	0.0021983	1.48
SiH3	0.0020903	1.41
H	0.0016399	1.10
C(CH3)3	0.0016448	1.11

Table S6. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [NHC(R)→ CuCl] complexes.

BSSE of [NHC(R)→ CuCl]		
R	E(HF)	E(Kcal.mol-1)
Br	0.002737	1.72
CF3	0.002938	1.84
Cl	0.002656	1.67
F	0.002514	1.58
CH_3	0.002928	1.84
Ph	0.003396	2.13
Si(CH3)3	0.004017	2.52
SiH3	0.002990	1.88
H	0.002603	1.63
C(CH3)3	0.003839	2.41

Table S7. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [NHC(R)→ CuOAc] complexes.

BSSE of [NHC(R)→ CuOAc]		
R	E(HF)	E(Kcal.mol-1)
Br	0.0025982	1.63
CF3	0.0022487	1.41
Cl	0.0025453	1.60
F	0.0020178	1.27
CH_3	0.0027545	1.73
Ph	0.0030831	1.93
Si(CH3)3	0.0034134	2.14
SiH3	0.0028360	1.78
H	0.0025729	1.61
C(CH3)3	0.0034123	2.14

Table S8. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [$P(Ph)_3$CHR→AgCl] complexes.

[P(Ph)3CHR→AgCl]		
R	E(HF)	E(Kcal.mol-1)
Br	0.002040	1.28
CF3	0.002610	1.64
Cl	0.002306	1.45
F	0.002330	1.46
CH_3	0.002385	1.50
Ph	0.002222	1.39
Si(CH3)3	0.002455	1.54
SiH3	0.002246	1.41
H	0.002312	1.45
C(CH3)3	0.002603	1.63

Table S9. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [$P(Ph)_3$CHR→AuCl] complexes.

[P(Ph)3CHR→AuCl]		
R	E(HF)	E(Kcal.mol-1)
Br	0.0017425	1.17
CF3	0.0022185	1.49
Cl	0.0019862	1.34
F	0.0020021	1.35
CH_3	0.0019861	1.34
Ph	0.0018629	1.25
Si(CH3)3	0.0020786	1.40
SiH3	0.0018332	1.23
H	0.0019881	1.34
C(CH3)3	0.0022077	1.48

Table S10. The values of basis set superposition error (BSSE) at the PBE/def2-TZVP level of theory for [$P(Ph)_3$CHR→CuCl] complexes.

[P(Ph)3CHR→CuCl]

R	E(HF)	E(Kcal.mo1)
Br	0.003764	2.53
CF3	0.004073	2.74
Cl	0.003979	2.68
F	0.003728	2.51
CH_3	0.003950	2.66
Ph	0.004011	2.70
Si(CH3)3	0.004256	2.86
SiH3	0.003856	2.59
H	0.003721	2.50
C(CH3)3	0.008180	2.81

Table S11: The uncorrected$^{\Delta E_{int}}$ (kcal mol^{-1}) with considering the BSSE values for [([NHC(R)→ MR′] and [{$P(Ph)_3$CHR}→MCl] (M = Cu(I), Ag(I), Au(I), R=F, Cl, Br ,CF_3, H, CH_3, $C(CH_3)_3$, $Si(CH_3)_3$, SiH_3, Ph, R′=Cl, OAc) at PBE/def2-TZVP level of theory.

Interaction Energies		[NHC(R)→ MCl]	[NHC(R)→ MOAC]	[{P(Ph)$_3$CHR}→MCl]
R	**M**	ΔE_{int} (kcal mol^{-1})		
	Cu	60.37	60.3	63.82
Br	**Au**	70.16	72.6	73.18
	Ag	48.21	46.75	51.9
	Cu	55.84	55.85	58.3
CF$_3$	**Au**	63.88	67.96	67.62
	Ag	42.88	40.1	47.57
	Cu	59.3	58.92	64.07
Cl	**Au**	69.03	71.29	73.76
	Ag	47.29	45.62	52.33
	Cu	53.53	53.84	67.21
F	**Au**	62.37	64.32	78.87
	Ag	41.97	40.35	56.35
	Cu	66.01	67.96	64.95
CH$_3$	**Au**	77.06	80.2	76.72
	Ag	54.6	54.72	55.1
	Cu	65.39	67.21	59.3
Ph	**Au**	75.8	79.13	71.7
	Ag	53.78	54.28	47.75
	Cu	68.02	70.16	62
Si(CH$_3$)$_3$	**Au**	79.38	83.77	69.31
	Ag	56.37	58.42	51.46
SiH$_3$	**Cu**	66.45	68.46	60.43

	Au	78	81.51	69.31
	Ag	54.36	54.78	49.7
	Cu	64.01	68.34	66.33
H	**Au**	75.24	77.87	76.76
	Ag	52.52	51.58	55.85
	Cu	63.32	65.57	63.19
$C(CH_3)_3$	**Au**	71.29	76.05	74.97
	Ag	48.51	48.88	53.84

Table S12: The uncorrected ΔE_{int} (kcal mol^{-1}) with considering the BSSE values for [([NHC(R)→ MCl] (M = Cu(I), Ag(I), Au(I), R=F, Cl, Br ,CF_3, H, CH_3, $C(CH_3)_3$, $Si(CH_3)_3$, SiH_3, Ph, R′=Cl, OAc) at PBE/def2-TZVP level of theory.

Interaction Energies(Kcalmol^{-1})		**[NHC(R)→ MCl]^a**	**[NHC(R)→MCl]^b**
R	**M**		
Br	**Cu**	-63.17	-64.41
	Au	-73.39	-74.71
	Ag	-51.18	-52.56
CF_3	**Cu**	-58.86	-59.62
	Au	-67.46	-67.90
	Ag	-45.99	-46.73

Cl	**Cu**	-61.95	-63.38
	Au	-72.08	-73.61
	Ag	-50.07	-51.69
F	**Cu**	-56.44	-58.07
	Au	-65.74	-67.45
	Ag	-44.97	-46.82
CH_3	**Cu**	-69.33	-70.79
	Au	-80.93	-82.85
	Ag	-58.17	-59.78
Ph	**Cu**	-67.62	-69.46
	Au	-77.79	-80.74
	Ag	-55.94	-58.21
$Si(CH_3)_3$	**Cu**	-73.41	-72.95
	Au	-85.73	-84.49
	Ag	-61.27	-60.75
SiH_3	**Cu**	-68.98	-70.15
	Au	-81.16	-82.27
	Ag	-57.23	-58.41
H	**Cu**	-67.53	-69.27

	Au	-79.27	-81.23
	Ag	-56.33	-58.21
$C(CH_3)_3$	**Cu**	-68.74	-67.92
	Au	-78.32	-77.35
	Ag	-57.54	-57.60

[a]NHC complexes bearing H atom on the non-carbenic carbon atoms in the heterocycle (C_3 and C_4, see scheme 1)

[b]NHC complexes bearing CH_3 group on the non-carbenic carbon atoms in the heterocycle (C_3 and C_4, see scheme 1)

Table S13: The natural hybrid orbital (NHO) analysis results of [NHC(R)→AgCl] complexes at PBE/def2-TZVP level of theory.

(Occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	**BOND**	**HYBRID**	**OCCUPANCY**
[NHC(Br)→AgCl]	Ag 1 - C 6	Ag1: $Sp^{1.2}d^{0.13}$	
		C6: $sp^{1.74}$	1.87273
	Ag 1 -Cl 9	Ag1: $sp^{0.97}d^{0.1}$	
		Cl9: $sp^{4.35}d^{0.02}$	1.93304
[NHC(CF3)→AgCl]	Ag 1 - C 6	Ag1: $Sp^{1.21}d^{0.11}$	
		Ag1: $Sp^{1.67}$	1.87677
	Ag 1 -Cl 9	Ag1: $Sp^{0.97}d^{0.09}$	
		Ag1: $Sp^{4.4}d^{0.02}$	1.94097
[NHC(Cl)→AgCl]	Ag 1 - C 6	Ag1: Sp1.2d0.13	1.87281
		C6: sp1.69	
	Ag 1 -Cl 9	Ag1: sp0.98d0.1	1.93564
		Cl9: sp4.37d0.02	
[NHC(F)→AgCl]	Ag 1 - C 6	Ag1: $Sp^{1.22}d^{0.13}$	1.84284
		C6: $sp^{1.79}$	
	Ag 1 -Cl 9	Ag1: $sp^{0.97}d^{0.09}$	1.93825
		Cl9: $sp^{4.6}d^{0.02}$	
[NHC(Me)→AgCl]	Ag 1 - C 6	Ag1: Sp1.17d0.13	1.87494
		C6: sp1.69	
	Ag 1 -Cl 9	Ag1: sp1.02d0.11	1.93597
		Cl9: $sp^{4.09}d^{0.01}$	
[NHC(Ph)→AgCl]	Ag 1 - C 6	Ag1: $Sp^{4.93}d^{0.02}$	No Data
		C6: $sp^{1.69}$	
	Ag 1 -Cl 9	Ag1: $sp^{1.02}d^{0.11}$	No Data
		Cl9: $sp^{4.09}d^{0.01}$	
[NHC(Si(CH3)3)→AgCl]	Ag 1 - C 6	Ag1: $Sp^{1.13}d^{0.11}$	1.86043
		C6: $sp^{1.74}$	
	Ag 1 -Cl 35	Ag1: $sp^{1.02}\,d^{0.19}$	1.93230
		Cl9: $sp^{3.46}\,d^{0.01}$	
[NHC(SiH3)→AgCl]	Ag 1 - C 6	Ag1: $Sp^{1.15}d^{0.12}$	1.87260
		C6: $sp^{1.65}$	
	Ag 1 -Cl 9	Ag1: $sp^{1.}\,d^{0.1}$	1.93417
		Cl9: $sp^{3.87}d^{0.01}$	
[NHC(H)→AgCl]	Ag 1 - C 6	Ag1: $sp^{1.17}d^{0.14}$	1.87854
		Cl9: $sp^{1.65}$	
	Ag 1 -Cl 9	Ag1: $Sp^{1.04}d^{0.1}$	1.93534
		C6: $sp^{4.51}\,d^{0.02}$	
[NHC(C(CH$_3$)$_3$)→AgCl]	Ag 34 - C 5	Ag34: $sp^{1.19}d^{0.1}$	1.86553
		C5: $sp^{1.78}$	
	Ag 34 -Cl 8	Ag34: $sp^{0.97}d^{0.09}$	1.94355
		Cl8: $sp^{3..5}d^{0.01}$	

Table S14: The natural hybrid orbital (NHO) analysis results of [NHC(R)→AgOAc] complexes at PBE/def2-TZVP level of theory.

(Occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	**BOND**	**HYBRID**	**OCCUPANCY**
[NHC(Br)→AgOAc]	Ag1-O4	Ag1: $Sp^{0.87}d^{0.1}$	
		O4: $sp^{1.74}$	1.89433
	Ag1-C8	Ag1: $sp^{1.34}d^{0.14}$	
		C8: $sp^{1.82}$	1.85585
[NHC(CF3)→AgOAc]	Ag1-O4	Ag1: $Sp^{2.06}d^{0.1}$	
		O4: $Sp^{12.57}d^{0.03}$	1.87200
	Ag1-C8	Ag1: $Sp1.65d^{0.1}$	
		C8:$SP^{1.66}$	1.86291
[NHC(Cl)→AgOAc]	Ag1-C6	Ag1: $Sp^{0.17}d^{0.09}$	1.94522
		C6: sp1.67	
	Ag1-O	-	No Data
		-	
[NHC(F)→AgOAc]	Ag1-O4	Ag1: $Sp^{0.89}d^{0.09}$	1.89729
		O4: $sp^{7.81}d^{0.01}$	
	Ag1-C8	Ag1: $sp^{1.34}d^{0.14}$	1.82539
		C8: $sp^{2.05}$	
[NHC(Me)→AgOAc]	Ag1-O4	Ag1: $Sp^{0.92}d^{0.11}$	1.89583
		O4: $sp^{7.2}d^{0.01}$	
	Ag1-C8	Ag1: $sp^{1.32}d^{0.14}$	1.85926
		C8: $sp^{1.72}$	
[NHC(Ph)→AgOAc]	Ag1-O4	-	No Data
		-	
	Ag1-C8	-	No Data
		-	
[NHC(Si(CH3)3)→AgOAc]	Ag1-C8	Ag1: $Sp^{1.08}$ $d^{0.12}$	1.93264
		C8: $sp^{1.78}$	
	Ag1-Cl 9	-	No Data
		-	
[NHC(SiH3)→AgOAc]	Ag1-O4	Ag1: $Sp^{0.91}$ $d^{0.11}$	1.89306
		O4: $sp^{6.88}$ $d^{0.01}$	
	Ag1-C8	Ag1: $sp^{1.32}$ $d^{0.14}$	1.85417
		C8: $sp^{1.70}d^{0.00}$	
[NHC(H)→AgOAc]	Ag1-O4	Ag1: $sp^{0.93}d^{0.11}$	1.89404
		O4: $sp^{7.65}$ $d^{0.01}$	
	Ag1-C8	Ag1: $Sp^{1.32}$ $d^{0.14}$	1.86232
		C8: $sp^{1.68}d^{0.00}$	
[NHC(C(CH3)3)→AgOAc]	Ag33-C5	Ag33: $sp^{1.36}d^{0.12}$	1.84701
		C5: $sp^{1.83}$	
	Ag33-O35	Ag33: $sp^{0.85}$ $d^{0.1}$	1.89986
		O35: $sp^{6.57}d^{0.00}$	

Table S15: The natural hybrid orbital (NHO) analysis results of [NHC(R)→AuCl] complexes at PBE/def2-TZVP level of theory.

(Occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	BOND	HYBRID	OCCUPANCY
[NHC(Br)→AuCl]	C 1 -Au 5	C_1: $Sp^{1.60}$	1.95906
		Au_5: $sp^{0.05}d^{0.25}$	
	Au5- Cl4	-	No Data
		-	
[NHC(CF3)→AuCl]	C 1 -Au 5	C_1: $Sp^{1.49}$	
		Au_5: $Sp^{0.06}d^{0.22}$	1.95850
	Au5- Cl4	-	
		-	No Data
[NHC(Cl)→AuCl]	C 1 -Au 5	C_1: $Sp^{1.60}$	1.96487
		Au_5: $sp^{0.05}d^{0.25}$	
	Au5- Cl4	-	No Data
		-	
[NHC(F)→AuCl]	C 1 -Au 5	C_1: $Sp^{1.47}$	1.95283
		Au_5: $Sp^{0.06}d^{0.22}$	
	Au5- Cl4	-	No Data
		-	
[NHC(Me)→AuCl]	C 1 -Au 5	C_1: $Sp^{1.60}$	1.96469
		Au_5: $Sp^{0.06}d^{0.23}$	
	Au5- Cl4	-	No Data
		-	
[NHC(Ph)→AuCl]	C 1 -Au 5	C_1: $Sp^{1.53}$	1.96236
		Au_5: $Sp^{0.06}d^{0.22}$	
	Au5- Cl4	-	No Data
		-	
[NHC(Si(CH3)3)→AuCl]	C 1 -Au 34	C_1: $Sp^{1.74}$	1.95131
		Au_{34}: $Sp^{0.05}d^{0.24}$	
	Au34-Cl35	-	No Data
		-	
[NHC(SiH3)→AuCl]	C 1 -Au 5	Au_5: $Sp^{0.06}d^{0.22}$	1.95590
		C_1: $sp^{1.61}$	
	Au5- Cl4	-	No Data
		-	
[NHC(H)→AuCl]	C 1 -Au 5	Au_5: $sp^{0.06}d^{0.24}$	1.96582
		C_1: $sp^{1.58}$	
	Au5- Cl4	-	No Data
		-	
[NHC(C(C(CH3)3)→AuCl]	C 1 -Au 5	Au_5: $sp^{1.16}d^{0.22}$	1.85189
		C_1: $sp^{1.63}$	
	Cl 4 -Au 5	Cl_4: $sp^{3.57}d^{0.01}$	1.90581
		Au5: $sp^{1.09}d^{0.21}f^{0.02}$	

Table S16: The natural hybrid orbital (NHO) analysis results of [NHC(R)→AuOAc] complexes at PBE/def2-TZVP level of theory.

(Occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	BOND	HYBRID	OCCUPANCY
[NHC(Br)→AuOAc]	C 5-Au 8	C_5: $Sp^{1.59}$	1.95906
		Au_8: $sp^{0.04}$ $d^{0.30}$	
	Au8-O9	-	-
		-	
[NHC(CF3)→AuOAc]	C 7 -Au 15	C_7: $Sp^{1.59}$	1.95216
		Au_{15}: $sp^{0.04}$ $d^{0.28}$	
	Au_{15}- O_3	-	-
		-	
[NHC(Cl)→AuOAc]	C 5 -Au 10	C_1: $Sp^{1.55}$	1.95811
		Au_5: $sp^{0.04}d^{0.30}$	
	Au_{10}- O_{11}	-	-
		-	
[NHC(F)→AuOAc]	C 5 -Au 8	C_1: $Sp^{1.56}$	**1.93902**
		Au_5: $Sp^{0.04}d^{0.29}$	
	Au8- O9	-	-
		-	
[NHC(Me)→AuOAc]	C 7 -Au 23	C_7: $Sp^{1.65}$	1.95912
		Au_{23}: $Sp^{0.04}d^{0.3}$	
	Au 23- O 3	-	-
		-	
[NHC(Ph)→AuOAc]	C 7 -Au 37	C_7: $Sp^{1.59}$	1.95563
		Au_{37}: $Sp^{0.04}d^{0.29}$	
	Au37- O3	-	-
		-	
[NHC(Si(CH3)3)→AuOAc]	C 7 -Au 41	C_1: $Sp^{1.64}$	2.00000
		Au_{34}: $Sp^{0.04}d^{0.3}$	
	Au41- O3	O3: $SP^{0.9}$ $d^{0.05}$	-
		Au_{34}: $Sp^{0.04}d^{0.3}$	
[NHC(SiH3)→AuOAc]	C 7 -Au 15	Au_{15}: $Sp^{0.04}d^{0.3}$	1.94871
		C_7: $sp^{1.68}$	
	Au15- O3	-	-
		-	
[NHC(H)→AuOAc]	C 5 -Au 8	Au_8: $Sp^{0.04}d^{0.31}$	1.96058
		C_5: $sp^{1.62}$	
	Au8- O9	-	-
		-	
[NHC(C(CH3)3)→AuOAc]	C 7 -Au 15	Au_{15}: $Sp^{0.05}d^{0.27}$	1.94342
		C_7: $sp^{1.71}$	
	Au15-O3	-	-
		-	

Table S17: The natural hybrid orbital (NHO) analysis results of [NHC(R)→CuCl] complexes at PBE/def2-TZVP level of theory.

(occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	BOND	HYBRID	OCCUPANCY
[NHC(Br)→CuCl]	C 1 -Cu 4	C_1: $Sp^{1.46}$	1.93165
		Cu_4: $Sp^{0.99}d^{0.08}$	
	Cu 4 - CL11	Cu_4: $sp^{1.14}d^{0.07}$	1.97506
		Cl_{11}: $Sp^{2.87}$ $d^{0.01}$	
[NHC(CF3)→CuCl]		C_1: $Sp^{1.41}$	1.93137
	C 1 -Cu 5	Cu_5: $sp^{1.01}d^{0.07}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.86}$ $d^{0.01}$	1.97853
		Cu_5: $sp^{1.11}d^{0.07}$	
[NHC(Cl)→CuCl]	C 1 -Cu 5	C_1: $Sp^{1.42}$	1.93136
		Cu_5: $sp^{0.99}d^{0.08}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.89}$ $d^{0.01}$	1.97512
		Cu_5: $sp^{1.14}d^{0.07}$	
[NHC(F)→CuCl]	C 1 -Cu 5	C_1: $Sp^{1.46}$	1.91373
		Cu_4: $Sp^{1.0}d^{0.08}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.97}$ $d^{0.01}$	1.97477
		Cu_5: $sp^{1.13}d^{0.07}$	
[NHC(Me)→CuCl]	C 1 -Cu 5	C_1: $Sp^{1.46}$	1.93204
		Cu_4: $Sp^{0.97}d^{0.09}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.79}$ $d^{0.01}$	1.97517
		Cu_5: $sp^{1.18}d^{0.08}$	
[NHC(Ph)→CuCl]	C 1 -Cu 5	-	-
		-	
[NHC(Si(CH3)3)→CuCl]	C 1 -Cu 4	C_1: $Sp^{1.47}$	1.93208
		Cu_4: $Sp^{0.94}d^{0.10}$	
	Cu 4 -Cl 35	Cu_4: $sp^{1.20}d^{0.07}$	1.97949
		Cl_{35}: $Sp^{2.56}$ $d^{0.01}$	
[NHC(SiH3)→AuCl]	C 1 -Cu 5	C_1: $Sp^{1.41}$	1.93205
		Cu_5: $Sp^{0.97}d^{0.08}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.71}$ $d^{0.01}$	1.97688
		Cu_5: $sp^{1.16}d^{0.07}$	
[NHC(H)→CuCl]	C 1 -Cu 5	C_1: $Sp^{1.44}$	1.93236
		Cu_5: $Sp^{0.98}d^{0.09}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.95}d^{0.01}$	
		Cu_5: $sp^{1.16}d^{0.08}$	1.97363
[NHC(C(CH3)3)→CuCl]	C 1 -Cu 5	C_1: $Sp^{1.46}$	1.92810
		Cu_5: $Sp^{0.98}d^{0.07}$	
	Cl 4 -Cu 5	Cl_4: $Sp^{2.46}d^{0.01}$	1.98205
		Cu_5: $sp^{1.15}d^{0.07}$	

Table S18: The natural hybrid orbital (NHO) analysis results of [NHC(R)→CuOAc] complexes at PBE/def2-TZVP level of theory.

(Occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	BOND	HYBRID	OCCUPANCY
[NHC(Br)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.53}$	1.89702
		Cu_4: $Sp^{1.13}$ $d^{0.11}$	
	Cu 4 - O 9	O_9: $Sp^{5.06}$	1.91890
		Cu_4: $sp^{1.05}$ $d^{0.12}$	
[NHC(CF3)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.36}$	1.94807
		Cu_4: $sp^{0.38}d^{0.05}$	
	Cu4- O17	-	
		-	-
[NHC(Cl)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.46}$	1.95307
		Cu_5: $sp^{0.24}d^{0.08}$	
	Cu4- O11	-	-
		-	
[NHC(F)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.49}$	1.92925
		Cu_4: $Sp^{0.32}d^{0.05}$	
	Cu4- O13	-	-
		-	
[NHC(Me)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.49}$	1.95584
		Cu_4: $Sp^{0.22}d^{0.09}$	
	Cu4- O17	-	-
		-	
[NHC(Ph)→CuOAc]	C 1 -Cu 4	-	-
		-	
	Cu 4- O 31	-	-
		-	
[NHC(Si(CH3)3)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.57}$	1.89616
		Cu_4: $Sp^{1.07}d^{0.10}$	
	Cu 4 - O 11	Cu_4: $Sp^{1.13}d^{0.12}$	1.92959
		O_{11}: $Sp^{3.92}$	
[NHC(SiH3)→CuOAc]	C 1 -Cu 4	Cu_{15}: $Sp^{0.04}d^{0.3}$	1.94871
		C_7: $sp^{1.68}$	
	Cu 4 - O 17	-	-
		-	
[NHC(H)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.53}$	1.95634
		Cu_4: $Sp^{0.24}d^{0.08}$	
	Cu4- O11	-	-
		-	
[NHC(C(CH3)3)→CuOAc]	C 1 -Cu 4	C_1: $Sp^{1.50}$	1.92074
		Cu_4: $Sp^{1.07}d^{0.08}$	
	Cu 4 - O 35	Cu_4: $Sp^{1.08}d^{0.10}$	1.94886
		O_{35}: $Sp^{3.02}$	

Table S19: The natural hybrid orbital (NHO) analysis results of [{$P(Ph)_3CH(R)$}→AgCl] complexes at PBE/def2-TZVP level of theory.

(**Occupancy**) **Bond orbital/ Coefficients/ Hybrids**			
COMPOUND	BOND	HYBRID	OCCUPANCY
[{$(Ph)_3PCHBr$}→AgCl]	C 1 -Ag 37	-	-
		-	
	Ag 37-Cl38	-	-
		-	
[{$(Ph)_3PCHCF3$}→AgCl]	C 1 -Ag 38	-	-
		-	
	Ag 38-Cl39	-	-
		-	
[{$(Ph)_3PCHCl$}→AgCl]	C 1 -Ag 37	-	-
		-	
	Ag 37-Cl38	-	-
		-	
[{$(Ph)_3PCHF$}→AgCl]	C 1 -Ag 37	C_1: $Sp^{3.08}d^{0.01}$	1.87992
		Ag_{37}: $Sp^{0.06}d^{0.11}$	
	-	-	-
		-	
[{$(Ph)_3PCHMe$}→AgCl]	C 1 -Ag 41	C_1: $Sp^{5.44}d^{0.01}$	1.82111
		Ag_{41}: $Sp^{0.03}d^{0.11}$	
	Ag 41-Cl42	-	-
		-	
[{$(Ph)_3PCHPPh$}→AgCl]	C 1 -Ag 37	C_1: $Sp^{7.41}d^{0.01}$	1.76555
		Ag_{37}: $Sp^{0.03}d^{0.10}$	
	Ag 37-Cl38	-	-
		-	
[{$(Ph)_3PCHSi(CH3)3$}→AgCl]	C 1 -Ag 37	C_1: $Sp^{7.69}$	1.82305
		Ag_{37}: $Sp^{0.01}d^{0.11}$	
	Ag 37-Cl38	-	-
		-	-
[{$(Ph)_3PCHSiH3$}→AgCl]	C 1 -Ag 37	C_1: $Sp^{7.50}d^{0.01}$	1.81258
		Ag_{37}: $Sp^{0.02}d^{0.10}$	
	Ag 37-Cl38	-	-
		-	
[{$(Ph)_3PCHH$}→AgCl]	C 1 -Ag 37	C_1: $Sp^{4.45}d^{0.01}$	1.86727
		Ag_{37}: $Sp^{0.05}d^{0.11}$	
	Ag 37-Cl38	-	-
		-	
[{$(Ph)_3PCHC(C(CH3)3$}→AgCl]	C 1 -Ag 38	C_1: $Sp^{5.77}d^{0.01}$	1.81128
		Ag_{38}: $Sp^{0.02}d^{0.10}$	
	Ag 37-Cl38	-	-
		-	

Table S20: The natural hybrid orbital (NHO) analysis results of [{$P(Ph)_3CH(R)$}→AuCl] complexes at PBE/def2-TZVP level of theory.

(Occupancy) Bond orbital/ Coefficients/ Hybrids			
COMPOUND	BOND	HYBRID	OCCUPANCY
[{$(Ph)_3PCHBr$}→AuCl]	C1- Au37	-	No Data
		-	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHCF3$}→AuCl]	C1- Au37	$C1:Sp^{3.84}$	1.88395
		$Au37:Sp^{0.02}d^{0.21}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHCl$}→AuCl]	Ag37-C1	-	No Data
		-	
	Ag37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHF$}→AuCl]	Au37-C 1	$C1:Sp^{2.73}d^{0.01}$	1.92952
		$Au37:Sp^{0.03}d^{0.23}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHMe$}→AuCl]	C1-Au41	$C1:SP^{4.31}D^{0.01}$	1.88360
		$Au41:SP^{0.02}D^{0.22}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHPPh$}→AuCl]	Au37-C 1	$C1:Sp^{4.23}d^{0.01}$	1.87834
		$Au37:Sp^{0.02}d^{0.21}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHSi(CH3)3$}→AuCl]	Au37-C 1	$C1:Sp^{5.54}d^{0.01}$	1.86913
		$Au37:Sp^{0.02}d^{0.2}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHSiH3$}→AuCl]	C1- Au37	$C1:Sp^{5.21}d^{0.01}$	1.87209
		$Au37:Sp^{0.2}d^{0.02}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHH$}→AuCl]	C1- Au37	$C1:S\ p^{3.57}d^{0.01}$	1.91985
		$Au37:Sp^{0.03}d^{0.22}$	
	Au37-Cl38	-	No Data
		-	
[{$(Ph)_3PCHC(C(CH3)3$}→AuCl]	Au38-C1	$C1:sp^{5.77}d^{0.01}$	1.81128
		$Au38:sp^{0.02}d^{0.1}$	
	Au38-Cl39	-	No Data
		-	

Table S21: The natural hybrid orbital (NHO) analysis results of [{$P(Ph)_3CH(R)$}→CuCl] complexes at PBE/def2-TZVP level of theory.

(**occupancy**) **Bond orbital/ Coefficients/ Hybrids**			
COMPOUND	BOND	HYBRID	OCCUPANCY
[{$(Ph)_3PCHBr$}→CuCl]	C1-Cu36	-	No Data
		-	
	Cu36-Cl37	-	No Data
		-	
[{$(Ph)_3PCHCF3$}→CuCl]	C 1 -Cu 36	C_1: $Sp^{4.39}$	1.83922
		Cu_{36}: $sp^{0.20}d^{0.10}$	
	Cu36-Cl37	-	No Data
		-	
[{$(Ph)_3PCHCl$}→CuCl]	C 1 -Cu 36	-	No Data
		-	
	Cu36-Cl37	-	No Data
		-	
[{$(Ph)_3PCHF$}→CuCl]	C 1 -Cu 36	C_1: $Sp^{2.76}$	1.88926
		Cu_{36}: $sp^{0.18}d^{0.10}$	
	Cu36-Cl37	-	No Data
		-	
[{$(Ph)_3PCHMe$}→CuCl]	C 1 -Cu 36	C_1: $sp^{4.79}d^{0.01}$	1.82823
		Cu_{36}: $sp^{0.18}d^{0.11}$	
	Cu36-Cl37	-	No Data
		-	
[{$(Ph)_3PCHPPh$}→CuCl]	C 1 -Cu 36	C_1: $Sp^{5.74}d^{0.01}$	1.79406
		Cu_{36}: $sp^{0.19}d^{0.10}$	
[{$(Ph)_3PCHSi(CH3)3$}→CuCl]	C 1 -Cu 50	C_1: $Sp^{6.69}d^{0.01}$	1.81568
		Cu_{50}: $sp^{0.21}d^{0.10}$	
	Cu 50-Cl51	No Data	No Data
		-	
[{$(Ph)_3PCHSiH3$}→CuCl]	C 1 -Cu 41	-	No Data
		-	
	Cu 41-Cl4	-	No Data
		-	
[{$(Ph)_3PCHH$}→CuCl]	C 1 -Cu 36	C_1: $Sp^{3.94}d^{0.01}$	1.87220
		Cu_{37}: $sp^{0.18}d^{0.10}$	
	Cu36-Cl37	-	No Data
		-	
[{$(Ph)_3PCHC(CH3)3$}→CuCl]	C 1 -Cu 36	C_1: $Sp^{4.96}d^{0.01}$	1.81761
		Cu_{36}: $sp^{0.20}d^{0.10}$	
	Cu36-Cl37	-	No Data
		-	

Complex	donor→Acceptor	Type	Values
[NHCCF3→CuOAc]	Cu 4 → C 1 - N 3	LP→σ*	20.08
[NHCC(CH3)3→CuOAc]	Cu 4 →C 1 - N 6	LP→σ*	8.93
[NHCCH3→CuOAc]	Cu 4 →C 1 - N 3	LP→σ*	9.55
[NHCCl→CuOAc]	Cu 4 →C 1 - N 3	LP→σ*	12.77
[NHCBr→CuOAc]	Cu 4 →C 1 - N 3	LP→σ*	12.03
[NHCF→CuOAc]	Cu 4 →C 1 - N 3	LP→σ*	17.09
[NHCSi(CH3)3→CuOAc]	Cu 4 → C 1 - N 3	LP→σ*	9.63
[NHCH→CuOAc]	Cu 4 →C 1 - N 3	LP→σ*	8.69
[NHCPh→CuOAc]	Cu 4 →C 1 - N 3	LP→σ*	10.39
[NHCSiH3→CuOAc]	Cu 4 → C 1 - N 3	LP→σ*	10.42

Table S22. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [NHC(R)→CuOAc] complexes at PBE/def2-TZVP level of theory.

Table S23. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [NHC(R)→AgOAc] complexes at PBE/def2-TZVP level of theory.

Complex	donor→Acceptor	Type	Values
[NHCCF3→AgOAc]	Ag 1 - O 4 →Ag 1 - C 8 Ag 1 → N 7 - C 8	σ→σ* LP→σ*	8.75 12.02
[NHCC(CH3)3→AgOAc]	Ag 33 - O 35 → C 5 -Ag 33 Ag 33→ N 3 - C 5 Ag 33 - O 35 → C 5 -Ag 33	σ →σ* LP→σ* σ* →σ*	17.00 5.71 3.91
[NHCCH3→AgOAc]	Ag 1 - O 4→ Ag 1 - C 8 Ag 1 - O 4→ Ag 1 - C 8	σ →σ* σ* →σ*	25.37 10.41
[NHCCl→AgOAc]	Ag 1 → N 4 - C 6	LP→σ*	10.24
[NHCBr→AgOAc]	Ag 1 - O 4 → Ag 1 - C 8 Ag 1 - O 4 → Ag 1 - C 8 Ag 1 → N 6 - C 8	σ →σ* σ* →σ* LP→σ*	24.84 10.48 8.81
[NHCF→AgOAc]	Ag 1 - O 4 → Ag 1 - C 8 Ag 1 - O 4 → Ag 1 - C 8	σ →σ* σ* →σ*	21.15 14.47
[NHCSi(CH3)3→AgOAc]	Ag 1 → N 6 - C 8	LP→σ*	7.07

[NHCH→AgOAc]	Ag 1 - O → Ag 1 - C 8 Ag 1 →N 6 - C 8 Ag 1 - O 4→ Ag 1 - C 8	σ →σ* LP→σ* σ →σ*	32.64 8.84 23.54
[NHCPh→AgOAc]	Ag 1 →N 6 - C 8	LP→σ*	7.68
[NHCSiH3→AgOAc]	Ag 1 - O 4 → Ag 1 - C 8 Ag 1 → N 6 - C 8 Ag 1 - O 4 → Ag 1 - C 8	σ →σ* LP→σ* σ →σ*	23.95 8.01 6.55

Table S24. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [NHC(R)→AuOAc] complexes at PBE/def2-TZVP level of theory.

Complex	**donor→Acceptor**	**Type**	**Values**
[NHCCF3→AuOAc]	Au 15 → C 7 -Au 15 Au 15 → C 7 -Au 15 Au 15 → N 5 - C 7 Au 15 → N 6 - C 7 Au 15 → N 5 - C 7	CR→σ* LP→σ* LP→σ* LP→σ* LP→σ*	5.55 3.84 4.28 4.56 18.70
[NHCC(CH3)3→AuOAc]	Au 15 → C 7 -Au 15 Au 15 → C 7 -Au 15 Au 15 → N 5 - C 7	CR→σ* LP→σ* LP→π*	5.35 4.96 12.65
[NHCCH3→AuOAc]	Au 23 → C 7 -Au 23 Au 23 → C 7 -Au 23 Au 23 → N 5 - C 7 Au 23 → N 6 - C 7 Au 23→ N 5 - C 7	CR→σ* LP→σ* LP→σ* LP→σ* LP→π*	6.25 3.36 3.72 3.93 15.12
[NHCCl→AuOAc]	Au 10 →C 5 -Au 10 Au 10 → C 5 -Au 10 Au 10 → N 3 - C 5 Au 10 → N 4 - C 5 Au 10 → N 3 - C 5	CR→σ* LP→σ* LP→π* LP→σ* LP→σ*	5.94 3.69 18.36 4.51 4.15
[NHCBr→AuOAc]	Au 8 → C 5 -Au 8 Au 8 → C 5 -Au 8 Au 8 → N 3 - C 5 Au 8 → N 4 - C 5 Au 8 →N 3 - C 5	CR→σ* LP→σ* LP→σ* LP→σ* LP→π*	5.87 3.81 4.01 4.29 17.59
[NHCF→AuOAc]	Au 8 → C 5 -Au 8 Au 8 →N 4 - C 5 Au 8 → N 3 - C 5 Au 8 → N 3 - C 5 Au 8 → N 4 - C 5	CR→σ* LP→σ* LP→π* LP→σ* LP→σ*	5.52 4.85 18.56 4.53 4.85

[NHCSi(CH3)3→AuOAc]	Au 41 → C 7 -Au 41 Au 41 → C 7 -Au 41 Au 41 → N 5 - C 7 Au 41 → N 6 - C 7 Au 41 → N 5 - C 7	CR→σ* LP→σ* LP→σ* LP→σ* LP→π*	5.91 4.45 3.52 3.01 14.09
[NHCH→AuOAc]	Au 8 → C 5 -Au 8 Au 8 → N 3 - C 5 Au 8 → N 4 - C 5 Au 8 → N 3 - C 5	CR→σ* LP→σ* LP→σ* LP→π*	6.41 4.15 4.50 17.31
[NHCPh→AuOAc]	Au 37 → C 7 -Au 37 Au 37 → C 7 -Au 37 Au 37 → N 5 - C 7 Au 37 → N 6 - C 7 Au 37 → N 5 - C 7	CR→σ* LP→σ* LP→σ* LP→σ* LP→π*	3.37 3.64 3.80 3.89 15.16
[NHCSiH3→AuOAc]	Au 15 → C 7 -Au 15 Au 15 → C 7 -Au 15 Au 15 → N 5 - C 7 Au 15 → N 5 - C 7	CR→σ* LP→σ* LP→σ* LP→π*	6.33 3.72 3.64 15.57

Table S25. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [NHC(R)→CuCl] complexes at PBE/def2-TZVP level of theory.

Complex	**donor→Acceptor**	**Type**	**Values**
[NHCCF3→CuCl]	Cl 4 -Cu 5 →C 1 -Cu 5 Cu 5 → C 1 - N 7	σ →σ* LP→π*	8.05 13.51
[NHCC(CH3)3→CuCl]	Cl 4 -Cu 5 → C 1 -Cu 5	σ →σ*	5.35
[NHCCH3→CuCl]	Cl 4 -Cu 5 → C 1 -Cu 5 Cu 5 → C 1 - N 7	σ →σ* LP→π*	9.92 9.18
[NHCCl→CuCl]	Cl 4 -Cu 5 → C 1 -Cu 5 Cu 5 → C 1 - N 3	σ →σ* LP→π*	9.61 11.97
[NHCBr→CuCl]	Cu 4 -Cl 11 → C 1 -Cu 4 Cu 4 →C 1 - N 3	σ →σ* LP→π*	9.24 11.37
[NHCF→CuCl]	Cl 4 -Cu 5 → C 1 -Cu 5 Cu 5 → C 1 - N 3	σ →σ* LP→π*	9.98 11.85
[NHCSi(CH3)3→CuCl]	Cu 4 -Cl 35 → C 1 -Cu 4	σ →σ*	7.40
[NHCH→CuCl]	Cl 4 -Cu 5 → C 1 -Cu 5 Cu 5 → C 1 - N 3	σ →σ* LP→π*	10.92 10.49

[NHCPh→CuCl]	-		
[NHCSiH3→CuCl]	Cl 4 -Cu 5 → C 1 -Cu 5 Cu 5 →C 1 - N 7	σ →σ* LP→π*	8.55 10.05

Table S26. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [NHC(R)→AgCl] complexes at PBE/def2-TZVP level of theory.

Complex	**donor→Acceptor**	**Type**	**Values**
[NHCCF3→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 → N 4 - C 6	σ →σ* LP→π*	25.70 8.54
[NHCC(CH3)3→AgCl]	Ag 34 → C 5 -Ag 34 Ag 34 → N 3 - C 5	σ →σ* LP→π*	16.61 5.57
[NHCCH3→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 →N 4 - C 6	σ →σ* LP→π*	26.50 7.20
[NHCCl→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 → N 4 - C 6	σ →σ* LP→π*	28.86 8.59
[NHCBr→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 →N 4 - C 6	σ →σ* LP→π*	27.86 8.26
[NHCF→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 →N 4 - C 6	σ →σ* LP→π*	23.33 8.49
[NHCSi(CH3)3→AgCl]	Ag 1 -Cl 35 → Ag 1 - C 6	σ →σ*	22.33
[NHCH→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 →N 5 - C 6	σ →σ* LP→π*	20.00 8.03
[NHCPh→AgCl]	-		
[NHCSiH3→AgCl]	Ag 1 -Cl 9 → Ag 1 - C 6 Ag 1 →N 4 - C 6	σ →σ* LP→π*	24.91 7.53

Table S27. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [NHC(R)→AuCl] complexes at PBE/def2-TZVP level of theory.

Complex	donor→Acceptor	Type	Values
[NHCCF3→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 -Au 5	LP→σ* CR→σ*	2.98 5.35
[NHCC(CH3)3→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7	CR→σ* LP→σ* LP→σ*	3.78 3.55 3.82
[NHCCH3→AuOAc]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7 Au 5 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	6.20 4.49 4.49 16.53
[NHCCl→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7 Au 5 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	5.97 5.24 5.24 20.68
[NHCBr→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3	CR→σ* LP→π*	6.00 16.10
[NHCF→AuOAc]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7 Au 5 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	5.54 5.52 5.52 20.55
[NHCSi(CH3)3→AuCl]	Au 34 → C 1 -Au 34 Au 34 → C 1 - N 3 Au 34 → C 1 - N 5 Au 34 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	 3.39 2.82 12.96
[NHCH→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7 Au 5 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	6.52 5.04 5.04 18.78
[NHCPh→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7 Au 5 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	6.00 4.63 4.6 17.86
[NHCSiH3→AuCl]	Au 5 → C 1 -Au 5 Au 5 → C 1 - N 3 Au 5 → C 1 - N 7 Au 5 → C 1 - N 3	CR→σ* LP→σ* LP→σ* LP→π*	6.37 4.46 3.16 17.73

Table S28. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [{$P(Ph)_3CH(R)$}→CuCl] complexes at PBE/def2-TZVP level of theory.

Complex	**donor→Acceptor**	**Type**	**Values**
[{$P(Ph)_3CHCF3$}→CuCl]	C 1 -Cu 36 →P 2 - C 25	σ →σ*	10.10
[{$P(Ph)_3CHC(CH3)3$}→CuCl]	C 1 -Cu 36 → P 2 - C 25	σ →σ*	14.69
[{$P(Ph)_3CHCH3$}→CuCl]	C 1 -Cu 36 → P 2 - C 25	σ →σ*	14.07
[{$P(Ph)_3CHCl$}→CuCl]	-	-	-
[{$P(Ph)_3CHBr$}→CuCl]	Cu 36 →C 1 -Br 38 Cu 36 →C 1 -Br 38	LP→σ* LP*→σ*	3.04 5.29
[{$P(Ph)_3CHF$}→CuCl]	C 1 -Cu 36 → P 2 - C 25	σ →σ*	8.70
[{$P(Ph)_3CHSi(CH3)3$}→CuCl]	C 1 -Cu 50 → P 2 - C 26	σ →σ*	14.17
[{$P(Ph)_3CHH$}→CuCl]	C 1 -Cu 37 → P 2 - C 26	σ →σ*	11.62
[{$P(Ph)_3CHPh$}→CuCl]	C 1 -Cu 36 → P 2 - C 25	σ →σ*	12.65
[{$P(Ph)_3CHSiH3$}→CuCl]	C 1 -Cu 41 → P 2 - C 26	σ →σ*	12.20

Table S29. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [{$P(Ph)_3CH(R)$}→AgCl] complexes at PBE/def2-TZVP level of theory.

Complex	donor→Acceptor	Type	Values
[{$P(Ph)_3CHCF3$}→AgCl]	C 1 -Ag 37 → P 2 - C 26	σ →σ*	12.42
[[{$P(Ph)_3CHC(CH3)3$}→AgCl]	C 1 -Ag 38 → P 2 - C 26	σ →σ*	15.15
[{$P(Ph)_3CHCH3$}→AgCl]	C 1 -Ag 41 →P 2 - C 26	σ →σ*	13.05
[{$P(Ph)_3CHCl$}→AgCl]	-	-	-
[{$P(Ph)_3CHBr$}→AgCl]	-	-	-
[{$P(Ph)_3CHF$}→AgCl]	C 1 -Ag 37 →P 2 - C 26	σ →σ*	8.22
[{$P(Ph)_3CHSi(CH3)3$}→AgCl]	C 1 -Ag 37 →P 2 - C 26	σ →σ*	10.86
[{$P(Ph)_3CHH$}→AgCl]	C 1 -Ag 37 → P 2 - C 26	σ →σ*	10.82
[{$P(Ph)_3CHPh$}→AgCl]	C 1 -Ag 37 → P 2 - C 26	σ →σ*	10.41
[{$P(Ph)_3CHSiH3$}→AgCl]	C 1 -Ag 37 →P 2 - C 26	σ →σ*	12.14

Table S30. The most important donor -acceptor interactions energy (kcal mol^{-1}) concern to M to C-N bond in [{$P(Ph)_3CH(R)$}→AuCl] complexes at PBE/def2-TZVP level of theory.

Complex	donor→Acceptor	Type	Values
[{$P(Ph)_3CHCF3$}→AuCl]	C 1 -Au 37 → P 2 - C 26 C 1 -Au 37 → C 39 - F 42	σ →σ* σ →σ*	13.96 9.73
[[{$P(Ph)_3CHC(CH3)3$}→AuCl]	C 1 -Au 37→ P 2 - C 26	σ →σ*	17.59
[{$P(Ph)_3CHCH3$}→AuCl]	C 1 -Au 41 →P 2 - C 26 Au 41 → C 1 -Au 41	σ →σ* CR→σ*	14.79 3.64
[{$P(Ph)_3CHCl$}→AuCl]	Au 37 → C 1 -Cl 39 Au 37 → C 1 - P 2	LP→σ* LP*→σ*	5.73 3.61
[{$P(Ph)_3CHBr$}→AuCl]	Au 37 → C 1 - P 2 Au 37 → C 1 - P 2 Au 37 → C 1 -Br 39	LP→σ* LP*→σ* LP*→σ*	3.28 4.96 15.11
[{$P(Ph)_3CHF$}→AuCl]	C 1 -Au 37 → P 2 - C 26	σ →σ*	8.63

[{$P(Ph)_3CHSi(CH3)3$}→AuCl]	C 1 -Au 37 → P 2 - C 26 Au 37 → C 1 -Au 37 Au 37 → C 1 -Au 37	σ →σ* CR→σ* LP→σ*	15.29 2.90 4.37
[{$P(Ph)_3CHH$}→AuCl]	C 1 -Au 38 → P 2 - C 26 Au 38 → C 1 - P 2	σ →σ* LP→σ*	10.82 3.21
[{$P(Ph)_3CHPh$}→AuCl]	C 1 -Au 37 → P 2 - C 25 Au 37 → C 1 -Au 37 Au 37 → C 1 -Au 37	σ →σ* CR→σ* LP→σ*	10.90 3.95 3.33
[{$P(Ph)_3CHSiH3$}→AuCl]	C 1 -Au 37 → P 2 - C 26 Au 37 → C 1 -Au 37	σ →σ* LP→σ*	13.63 5.05

Table S31. Topological properties critical points of bond of [NHC(R) → MR′] and [{$P(Ph)_3CHR$}→MCl] { M=Cu(I), Au(I) and Ag(I) , R= Br, CF3, Cl, F, Me, Ph, Si(Ch3)3,SiH3, H, C(CH3)3} complexes at PBE/def2-TZVP level of theory.

	Carben-M-CL			Carben-M-OAC			Ylide-M-CL		
R	**ρ(rc)**	**Δ^2ρ(rc)**	**-G/V**	**ρ(rc)**	**Δ^2ρ(rc)**	**-G/V**	**ρ(rc)**	**Δ^2ρ(rc)**	**-G/V**
Br	0.1298	0.3674	0.7068	0.1326	0.3662	0.7015	0.1162	0.2836	0.7003
CF3	0.1291	0.3767	0.7116	0.1344	0.3887	0.7057	0.1055	0.2471	0.7042
Cl	0.1231	0.3347	0.7076	0.1334	0.3681	0.7008	0.1147	0.2767	0.7001
F	0.1299	0.3605	0.7028	0.1349	0.3622	0.6945	0.1171	0.2770	0.6964
Me	0.1284	0.3420	0.7007	0.1320	0.3387	0.6931	0.1074	0.2326	0.6929
Ph	0.1284	0.3505	0.7038	0.1313	0.3460	0.6971	0.1048	0.2316	0.6970
Si(CH3)3	0.1284	0.3381	0.6997	0.1314	0.3326	0.6922	0.1038	0.2277	0.6977
SiH3	0.1295	0.3486	0.7016	0.1295	0.3485	0.7016	0.1054	0.2344	0.6975
H	0.1308	0.3594	0.7028	0.1314	0.3261	0.6872	0.1103	0.2431	0.6921
C(CH3)3	0.1231	0.3347	0.7076	0.1268	0.3342	0.7007	0.1062	0.2283	0.6928
Br	0.1537	0.2852	0.6509	0.1595	0.2760	0.6400	0.1353	0.2120	0.6459
CF3	0.1517	0.2979	0.6586	0.1591	0.2861	0.6443	0.1214	0.1921	0.6574
Cl	0.1542	0.2894	0.6517	0.1601	0.2800	0.6406	0.1338	0.2070	0.6458
F	0.1530	0.2908	0.6531	0.1590	0.2811	0.6416	0.1384	0.2049	0.6385
Me	0.1509	0.2586	0.6445	0.1576	0.2472	0.6314	0.1597	0.1758	0.6432
Ph	0.1518	0.2674	0.6469	0.1573	0.2573	0.6358	0.1242	0.1842	0.6476
Si(CH3)3	0.1507	0.2452	0.6395	0.1575	0.2311	0.6252	0.1178	0.1632	0.6455
SiH3	0.1536	0.2562	0.6401	0.1594	0.2423	0.6274	0.1199	0.1780	0.6512
H	0.1545	0.2747	0.6461	0.1608	0.2648	0.6344	0.1274	0.1768	0.6384
C(CH3)3	0.1432	0.2526	0.6529	0.1487	0.2391	0.6393	0.1200	0.1622	0.6419
Br	0.1141	0.3448	0.7650	0.1165	0.3420	0.7577	0.0994	0.2655	0.7675
CF3	0.1100	0.3444	0.7758	0.1138	0.3555	0.7696	0.0897	0.2303	0.7734
Cl	0.1140	0.34784	0.7650	0.1160	0.3382	0.7556	0.0988	0.2605	0.7665
F	0.1136	0.3417	0.7628	0.1160	0.3382	0.7556	0.1026	0.2658	0.7599
Me	0.1135	0.3251	0.7586	0.1175	0.3252	0.7489	0.0933	0.2236	0.7581
Ph	0.1128	0.3292	0.7624	0.1156	0.3269	0.7543	0.0889	0.2151	0.7626
Si(CH3)3	0.1122	0.3147	0.7579	0.1163	0.3159	0.7485	0.0895	0.2061	0.7365
SiH3	0.1137	0.3288	0.7604	0.1173	0.3281	0.7515	0.0895	0.2061	0.7365
H	0.1157	0.3408	0.7601	0.1191	0.3418	0.7521	0.0962	0.2347	0.7564
C(CH3)3	0.1040	0.2976	0.7698	0.1075	0.2960	0.7596	0.0893	0.2115	0.7618

Table 32. EDA analysis (BP86-D3/TZ2P(ZORA)//PBE/def2-TZVP) of the [([NHC(R)→ MCl] bearing H atom on the non-carbenic carbon atoms (R=F, Cl, Br ,CF_3, H, CH_3, $C(CH_3)_3$, $Si(CH_3)_3$, SiH_3, Ph, R′=Cl, OAc) with the C1 symmetry.

R		[NHC (R)→ CuCl]	[NHC (R)→ AgCl]	[NHC (R)→ AuCl]	R		[NHC (R)→ CuCl]	[NHC (R)→ AgCl]	[NHC (R)→ AuCl]
	ΔE int	-69.64	-55.43	-79.56		**ΔE int**	-76.66	-59.97	-84.63
	ΔEpauli	110.35	122.65	197.61		**ΔEpauli**	120.52	129.77	206.70
Br	**ΔEelast**	-126.16(70.16)	-127.70(71.71)	-194.60(70.21)	**Ph**	**ΔEelast**	-139.52(70.75)	-139.00(73.25)	-209.10(71.77)
	ΔEorb	-49.43(27.49)	-43.59(24.48)	-74.88(27.02)		**ΔEorb**	-50.01(25.36)	-43.72(23.04)	-73.82(25.34)
	ΔEdisper	-4.22(2.34)	-6.78(3.81)	-7.68(2.77)		**ΔEdisper**	-7.66(3.88)	-7.03(3.70)	-8.41(2.89)
	ΔE int	-64.48	-48.10	-71.23		**ΔE int**	-86.32	-67.10	-95.19
	ΔEpauli	113.53	120.72	197.96		**ΔEpauli**	132.79	147.38	230.56
	ΔEelast	-124.2(69.77)	-121.92(72.22)	-189.87(70.54)		**ΔEelast**	-157.61(71.93)	-160.24(74.71)	-239.17(73.41)
	ΔEorb	-49.39(7.74)	-41.55(24.61)	-73.31(27.23)		**ΔEorb**	-49.50(22.59)	-44.72(20.85)	-74.76(22.95)
CF3	**ΔEdisper**	-4.40(2.47)	-5.35(3.17)	-6.00(2.23)	**Si(CH3)3**	**ΔEdisper**	-12.00(5.47)	-9.51(4.43)	-11.88(3.65)
	ΔE int	-67.76	-53.13	-76.36		**ΔE int**	-77.90	-60.42	-86.47
	ΔEpauli	109.53	121.33	195.59		**ΔEpauli**	124.99	139.07	221.97
	ΔEelast	-124.78(70.38)	-126.13(72.30)	-192.11(70.64)		**ΔEelast**	-146.71(72.31)	-149.86(75.12)	-226.49(73.43)
	ΔEorb	-48.56(27.39)	-42.53(24.38)	-73.72(27.11)		**ΔEorb**	-48.99(24.14)	-43.48(21.80)	-74.79(24.25)
Cl	**ΔEdisper**	-3.95(2.22)	-5.80(3.32)	-6.13(2.25)	**SiH3**	**ΔEdisper**	-7.18(3.53)	-6.15(3.08)	-7.16(2.32)
	ΔE int	-61.11	-45.80	-67.85		**ΔE int**	-72.99	-56.72	-81.10
	ΔEpauli	100.94	111.46	180.28		**ΔEpauli**	117.60	133.84	21.63
	ΔEelast	-111.39(68.73)	-112.66(71.63)	-172.52(69.53)		**ΔEelast**	-142.40(74.71)	-146.80(77.03)	-218.81(74.75)
	ΔEorb	-47.60(29.37)	-41.12(26.15)	-71.64(28.87)		**ΔEorb**	-44.79(23.50)	-40.67(21.34)	-70.26(24.00)
F	**ΔEdisper**	-3.06(1.88)	-3.49(2.22)	-3.96(1.60)	**H**	**ΔEdisper**	-3.40(1.78)	-3.10(1.63)	-3.66(1.25)
	ΔE int	-76.56	-59.85	-84.86		**ΔE int**	-79.23	-	-85.84
	ΔEpauli	120.44	135.82	213.41		**ΔEpauli**	131.39	-	218.87
	ΔEelast	-145.18(73.69)	-149.08(76.19)	-221.02(74.15)		**ΔEelast**	-149.74(71.09)	-	-220.93(72.51)

	ΔEorb	-46.46(23.58)	-42.14(21.54)	-71.73(24.06)		**ΔEorb**	-51.59(24.49)	-	-74.77(24.54)
Me	**ΔEdisper**	-5.36(2.72)	-4.44(2.27)	-5.32(1.78)	**C(CH3)3**	**ΔEdisper**	-9.28(4.40)	-	-9.01(2.96)

Table 33. EDA analysis (BP86-D3/TZ2P(ZORA)//PBE/def2-TZVP) of the [([NHC(R)→ MCl] bearing CH_3 atom on the non-carbenic carbon atoms (R=F, Cl, Br ,CF_3, H, CH_3, $C(CH_3)_3$, $Si(CH_3)_3$, SiH_3, Ph, R′=Cl, OAc) with the C1 symmetry.

R		[NHC (R) CuCl]	[NHC (R)→ AgCl]	[NHC (R)→ AuCl]	R		[NHC (R)→ CuCl]	[NHC (R)→ AgCl]	[NHC (R)→ AuCl]
	ΔE int	-70.64	-56.86	-80.85		**ΔE int**	-78.81	-62.74	-87.47
	ΔEpauli	110.96	122.85	197.86		**ΔEpauli**	118.49	130.57	206.95
Br	**ΔEelast**	-128.26(70.63)	-129.47(72.04)	-196.44(79.63)	**Ph**	**ΔEelast**	-140.30 (71.11)	-142.25 (72.56)	-212.17 (72.06)
	ΔEorb	-49.07(27.02)	-43.34(24.12)	-43.34(17.57)		**ΔEorb**	-49.14 (24.90)	-49.39 (25.19)	-73.45 (24.95)
	ΔEdisper	-4.26(2.35)	-6.90(3.84)	-6.90(2.8)		**ΔEdisper**	-7.87 (3.99)	-4.40 (2.24)	-8.80 (2.99)
	ΔE int	-65.22	-48.89	-71.78		**ΔE int**	-85.78	-66.93	-93.87
	ΔEpauli	-115.12	120.17	197.99		**ΔEpauli**	139.89	153.35	238.15
	ΔEelast	-126.96(70.4)	-122.82(72.65)	-191.29(70.91)		**ΔEelast**	-161.89(71.74)	-164.23(74.56)	-244.06(73.51)
	ΔEorb	-48.95(27.14)	-40.86(24.17)	-72.36(26.82)		**ΔEorb**	-51.43(22.79)	-46.10(20.93)	-76.18(22.94)
CF3	**ΔEdisper**	-4.43(2.46)	-5.38(3.18)	-6.12(2.27)	**Si(CH3)3**	**ΔEdisper**	-12.35(5.47)	-9.94(4.51)	-11.79(3.55)
	ΔE int	-69.18	-54.83	-77.95		**ΔE int**	-79.04	-61.45	-87.51
	ΔEpauli	110.14	122.34	196.85		**ΔEpauli**	126.83	140.40	224.97
	ΔEelast	-127.20(70.93)	-128.91(72.76)	-195.24(71.05)		**ΔEelast**	-149.66(72.7)	-152.23(75.42)	-230.30(73.7)
	ΔEorb	-48.11(26.83)	-42.35(23.9)	-73.32(26.68)		**ΔEorb**	-48.99(23.8)	-43.47(21.54)	-74.97(23.99)
Cl	**ΔEdisper**	-4.01(2.24)	-5.91(3.34)	-6.23(2.27)	**SiH3**	**ΔEdisper**	-7.22(3.51)	-6.14(3.04)	-7.21(2.31)
	ΔE int	-62.76	-47.74	-69.62		**ΔE int**	-74.73	-58.58	-83.11
	ΔEpauli	101.24	112.03	180.95		**ΔEpauli**	119.12	135.87	214.87
	ΔEelast	-113.96(69.49)	-115.46(72.27)	-175.61(70.08)		**ΔEelast**	-145.94(75.29)	-150.47(77.49)	-224.16(75.23)
	ΔEorb	-46.90(28.6)	-40.73(25.49)	-70.92(28.3)		**ΔEorb**	-44.41(22.91)	-40.52(20.87)	-70.05(23.51)

F	**ΔEdisper**	-3.14(1.91)	-3.58(2.24)	-4.07(1.62)	**H**	**ΔEdisper**	-3.49(1.8)	-3.19(1.64)	-3.77(1.27)
	ΔE int	-78.06	-61.49	-86.34		**ΔE int**	-78.17	-62.65	-85.52
	ΔEpauli	121.88	138.10	215.46		**ΔEpauli**	137.99	140.05	218.03
	ΔEelast	-148.33(74.18)	-152.90(76.61)	-224.96(74.54)		**ΔEelast**	-152.76(70.67)	-149.17(73.59)	-217.60(71.64)
	ΔEorb	-46.19(23.10)	-42.17(21.13)	-71.44(23.67)		**ΔEorb**	-54.14(25.05)	-45.58(22.49)	-76.27(25.11)
Me	**ΔEdisper**	-5.43(2.72)	-4.51(2.26)	-5.40(1.79)	**C(CH3)3**	**ΔEdisper**	-9.26(4.28)	-7.96(3.93)	-9.86(3.25)

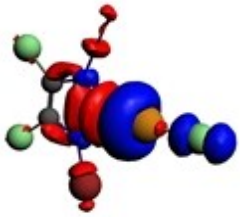
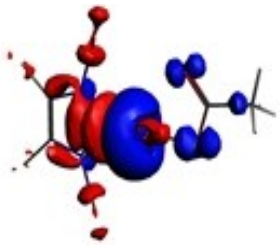
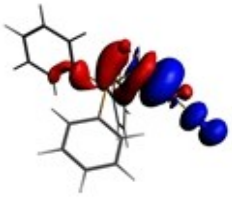
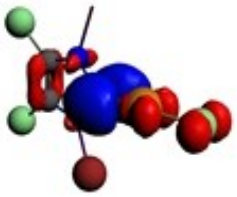
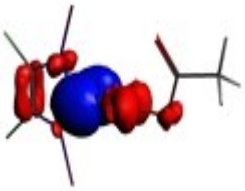
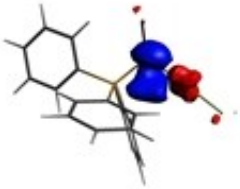
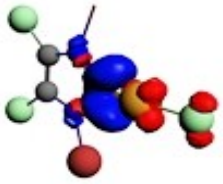
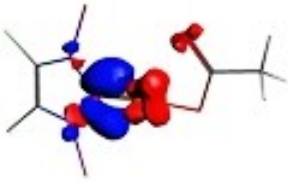
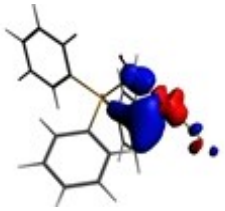
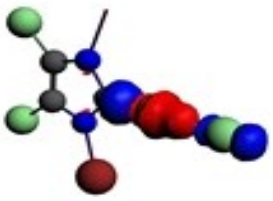
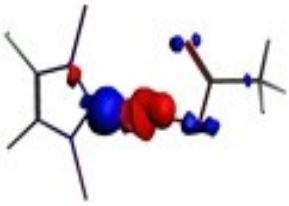
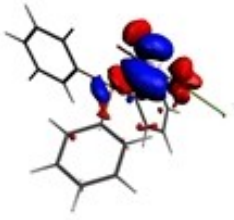
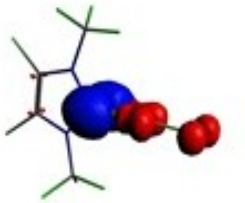
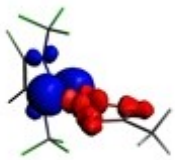
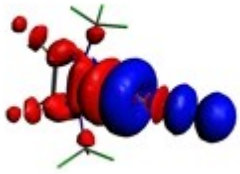
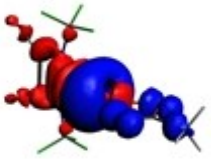
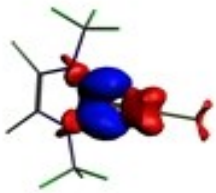
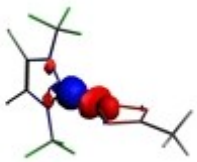
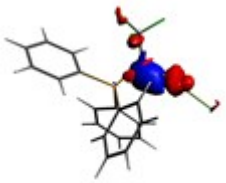
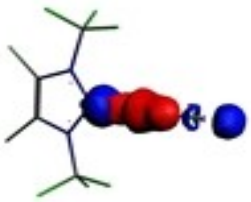
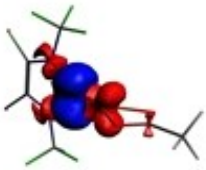
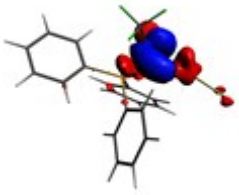
[NHC(Br)→CuCl]	[NHC(Br)→CuOAC]	[{(Ph)$_3$PCHBr}→CuCl]
		
Δρ1: ΔE =-21.35, ν = 0.43 Contour =0.001	Δρ1: ΔE =-21.59, ν = 0.37 Contour =0.001	Δρ1: ΔE =-26.08, ν = 0.48 Contour =0.001
		
Δρ2: ΔE =-12.07, ν =0.38 Contour =0.005	Δρ2: ΔE =-12.48, ν =0.38 Contour =0.001	Δρ2: ΔE =-7.66, ν = 0.30 Contour =0.001
		
Δρ3: ΔE =-5.45, ν = 0.21 Contour =0.005	Δρ3: ΔE =-5.92, ν =0.20 Contour =0.0005	Δρ3: ΔE =-6.81, ν = 0.22 Contour =0.0005
		
Δρ4: ΔE =-5.29, ν = 0.15 Contour =0.003	Δρ4: ΔE =-6.22, ν = 0.17 Contour =0.0005	Δρ4: ΔE =0.16, ν = -3.83 Contour =0.0005
Δρ rest: ΔE = -2.95	Δρ rest: ΔE = -3.32	Δρ rest: ΔE = -8.16

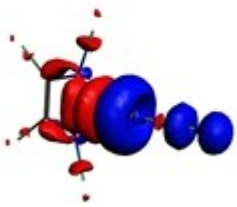
Fig. S1. Deformation densities associated with the most important orbital interactions for [NHC(Br)→CuR′] And [{P(Ph)$_3$CHBr}←CuCl](R′=Cl, OAc) complexes.

[NHC(CF3)→CuCl]	**[NHC(CF3)→CuOAC]**	**[{(Ph)$_3$PCHCF3}→CuCl]**
		
Δρ1: ΔE =-14.59, ν = 0.46 Contour =0.001	Δρ1: ΔE =-22.52, ν = 0.57 Contour =0.001	Δρ1: ΔE =-25.54, ν =0.47 Contour =0.001
		
Δρ2: ΔE =-18.87, ν = 0.37 Contour =0.0005	Δρ2: ΔE =-17.79, ν = 0.39 Contour =0.0005	Δρ2: ΔE =-7.49, ν = 0.25 Contour =0.001
		
Δρ3: ΔE =-5.29, ν = 0.17 Contour =0.0005	Δρ3: ΔE =-8.82, ν =0.19 Contour =0.0007	Δρ3: ΔE =-4.3, ν = 0.17 Contour =0.0005
		
Δρ4: ΔE =-5.16, ν =0.14 Contour =0.0003	Δρ4: ΔE =-5.49, ν = 0.17 Contour =0.0003	Δρ4: ΔE =-3.1, ν = 0.14 Contour =0.0003

Δρ rest: ΔE = -2.55 Δρ rest: ΔE = -1.63 Δρ rest: ΔE = -6.05

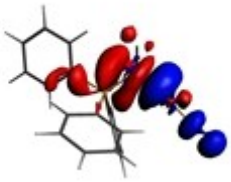
Fig. S2. Deformation densities associated with the most important orbital interactions for [NHC(CF3)→CuR′] And [{P(Ph)$_3$CHCF3}→CuCl](R′=Cl, OAc) complexes.

[NHC(Cl)→Cl] **[NHC(Cl)→CuOAC]** **[{(Ph)$_3$PCHCl}→CuCl]**

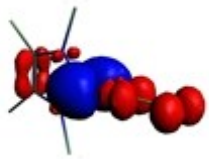


Δρ1: ΔE =-20.39, ν = 0.41
Contour =0.001

-

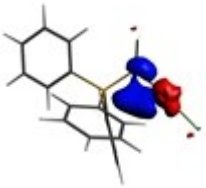


Δρ1: ΔE = -26.55 ν = 0.48
Contour =0.001

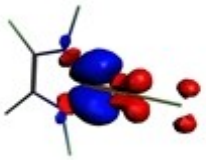


Δρ2: ΔE =-12.68, ν =0.40
Contour =0.0005

-

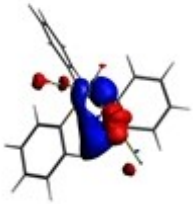


Δρ2: ΔE =-7.72 ν =0.28
Contour =0.001

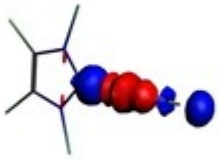


Δρ3: ΔE =-5.56, ν = 0.2
Contour =0.0005

-

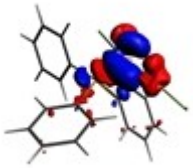


Δρ3: ΔE =-5.97, ν = 0.21
Contour =0.0005



Δρ4: ΔE =-5.38, ν = 0.15
Contour =0.0003

-



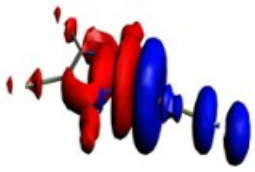
Δρ4: ΔE = -3.7, ν = 0.16
Contour =0.0003

Δρ rest: ΔE = -2.26

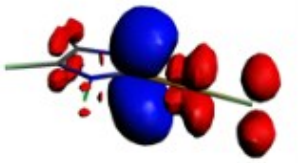
Δρ rest: ΔE = -6.18

Fig. S3. Deformation densities associated with the most important orbital interactions for [NHC(Cl)→CuR′] and [{P(Ph)$_3$CHCl}→CuCl](R′=Cl, OAc) complexes.

[NHC(F)→CuCl]



Δρ1: ΔE= -20.49, ν= 0.4
Contour=0.001

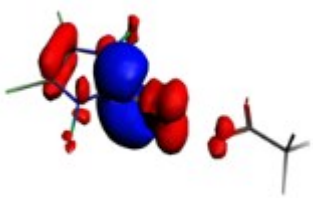


Δρ2: ΔE= -11.86, ν= 0.0.39
Contour=0.0005

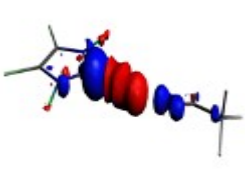
Δρ3: ΔE= -6.14, ν= 0.19
Contour=0.0005

[NHC(F)→CuOAC]

Δρ1: ΔE= -20.94, ν= 0.43
Contour=0.001

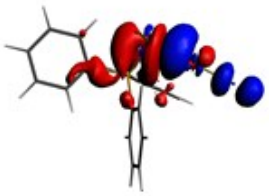


Δρ2: ΔE= -12.17, ν= 0.0.37
Contour=0.0005

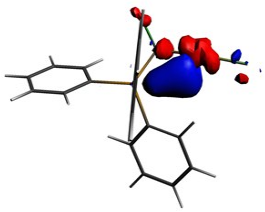


Δρ3: ΔE= -11.11, ν= 0.28
Contour=0.0005

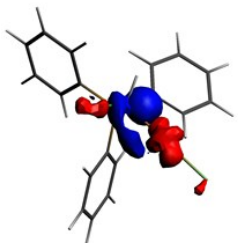
[{(Ph)$_3$PCHF}→CuCl]



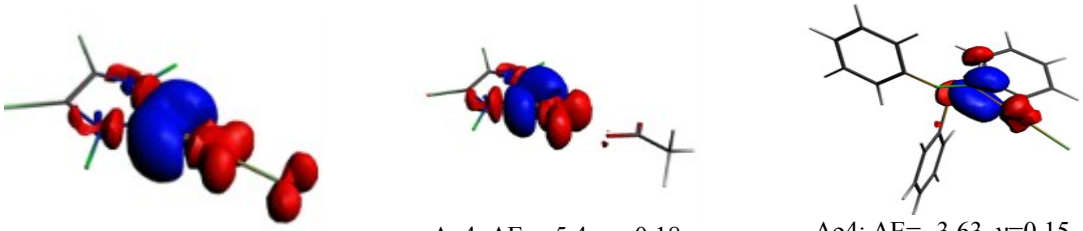
Δρ1: ΔE= -28.46, ν= 0.52
Contour=0.001



Δρ2: ΔE= -8.06, ν= 0.28
Contour=0.001



Δρ3: ΔE= -5.80, ν=0.22
Contour=0.0005



Δρ4: ΔE= -5.39, ν= 0.18
Contour=0.0003

Δρ rest: ΔE= -1.49

Δρ4: ΔE= -5.4, ν= 0.18
Contour=0.0003

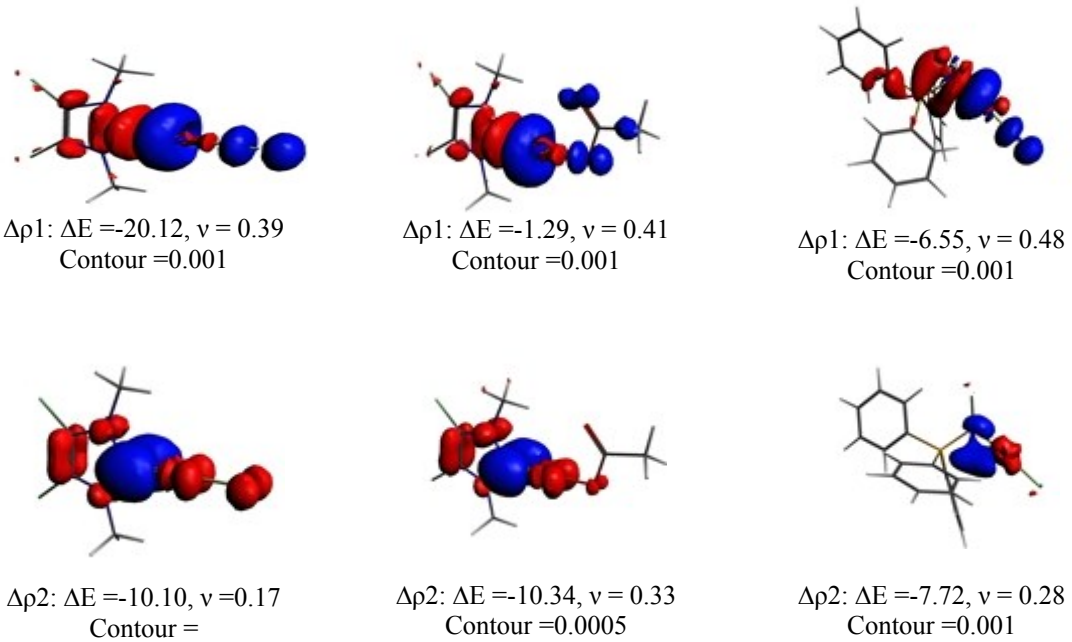
Δρ rest: ΔE= -2.06

Δρ4: ΔE= -3.63, ν=0.15
Contour=0.0005

Δρ rest: ΔE= -6.99

Fig. S4. Deformation densities associated with the most important orbital interactions for [NHC(F)→CuR′] And [{P(Ph)$_3$CHF}→CuCl](R′=Cl, OAc) complexes.

[NHC(Me)→CuCl] **[NHC(Me)→CuOAC]** **[{(Ph)$_3$PCHMe}→CuCl]**



Δρ1: ΔE =-20.12, ν = 0.39
Contour =0.001

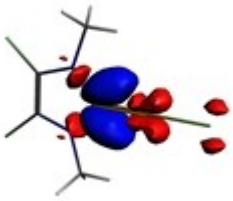
Δρ1: ΔE =-1.29, ν = 0.41
Contour =0.001

Δρ1: ΔE =-6.55, ν = 0.48
Contour =0.001

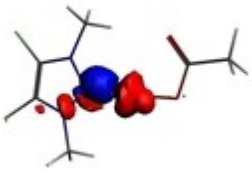
Δρ2: ΔE =-10.10, ν =0.17
Contour =

Δρ2: ΔE =-10.34, ν = 0.33
Contour =0.0005

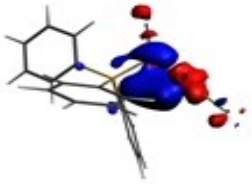
Δρ2: ΔE =-7.72, ν = 0.28
Contour =0.001



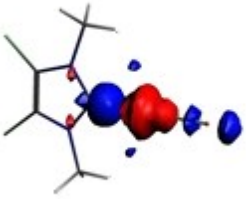
Δρ3: ΔE =-4.72, ν = 0.17
Contour =



Δρ3: ΔE =-7.20, ν =0.19
Contour =0.005

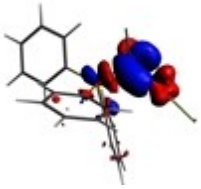


Δρ3: ΔE =,-5.97 ν = 0.21
Contour =0.0005



Δρ4: ΔE =-5.59, ν = 0.16
Contour =

Δρ4: ΔE =-4.6, ν =0.15
Contour =0.0003



Δρ4: ΔE =-3.76, ν =0.16
Contour =0.0003

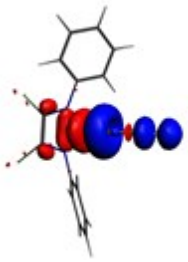
Δρ rest: ΔE = -2.96

Δρ rest: ΔE = -4.48

Δρ rest: ΔE = -6.18

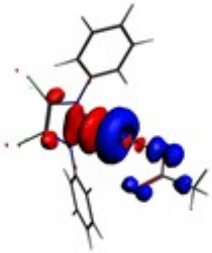
Fig. S5. Deformation densities associated with the most important orbital interactions for [NHC(CH3)→CuR′] And [{P(Ph)$_3$CHCH3}→CuCl](R′=Cl, OAc) complexes.

[NHC(Ph)→CuCl]



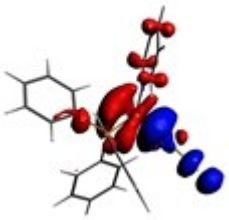
Δρ1: ΔE =-020.12, ν = 0.39
Contour =

[NHC(Ph)→CuOAC]

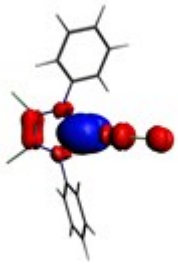


Δρ1: ΔE =-21.07, ν = 0.41
Contour =0.001

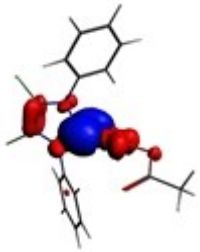
[{(Ph)$_3$PCHPh}→CuCl]



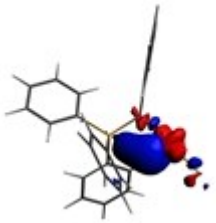
Δρ1: ΔE =-27.57, ν = 0.51
Contour =0.001



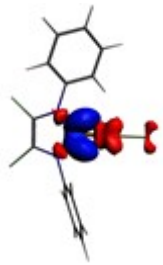
Δρ2: ΔE =-11.61, ν = 0.37
Contour =



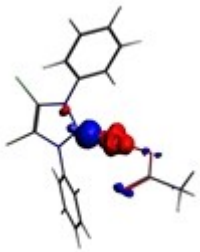
Δρ2: ΔE =-12.05, ν =0.36
Contour =0.0005



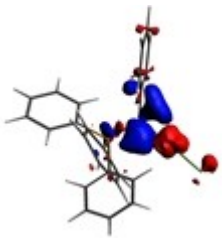
Δρ2: ΔE =-7.91, ν =0.27
Contour =0.0005



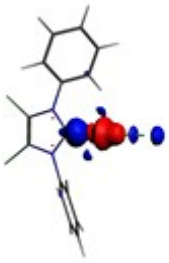
Δρ3: ΔE =-4.79, ν = 0.17
Contour =



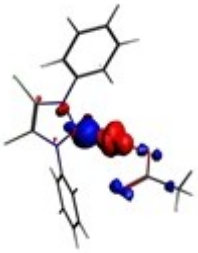
Δρ3: ΔE =-6.44, ν = 0.18
Contour =0.0005



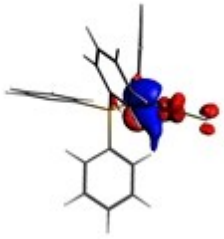
Δρ3: ΔE =-3.80, ν = 0.18
Contour =0.0003



Δρ4: ΔE =-5.51, ν = 0.16
Contour =



Δρ4: ΔE =-5.01, ν = 0.17
Contour =0.0003



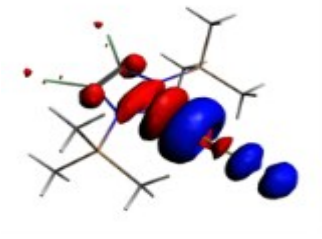
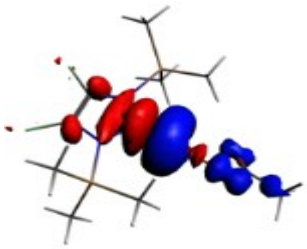
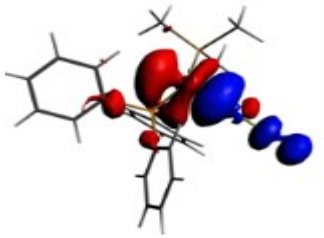
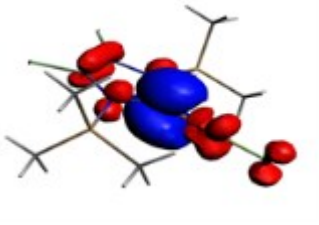
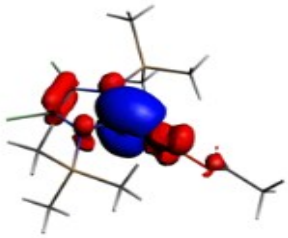
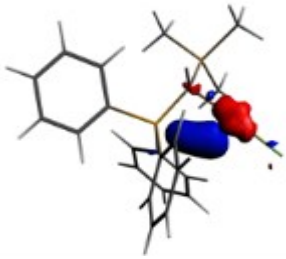
Δρ4: ΔE =-3.28, ν = 0.15
Contour =0.0003

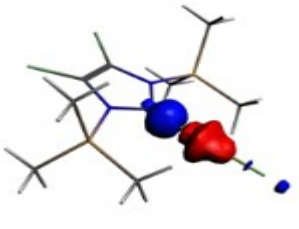
Δρ rest: ΔE = -3.98

Δρ rest: ΔE = -5.57

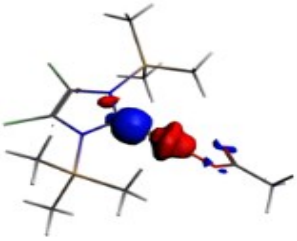
Δρ rest: ΔE = -8.77

Fig. S6. Deformation densities associated with the most important orbital interactions for [NHC(Ph)→CuR′] And [{P(Ph)$_3$CHPh}→CuCl](R′=Cl, OAc) complexes.

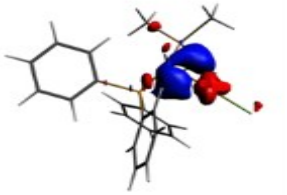
[NHC(Si(CH3)3)→CuCl]	**[NHC(Si(CH3)3)→CuOAC]**	**[{(Ph)$_3$PCH Si(CH3)3}→CuCl]**
		
Δρ1: ΔE= -23.9, ν= 0.41 Contour=0.001	Δρ1: ΔE= -24.91, ν= 0.43 Contour=0.001	Δρ1: ΔE= -26.12, ν= 0.47 Contour=0.001
		
Δρ2: ΔE= -10.84, ν= 0.0.35 Contour=0.0005	Δρ2: ΔE= -11.70, ν= 0.0.35 Contour=0.0005	Δρ2: ΔE= -8.10, ν= 0.27 Contour=0.001



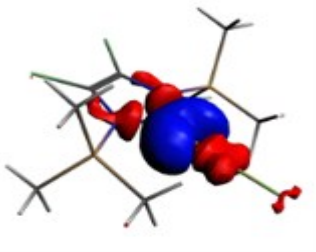
Δρ3: ΔE= -4.52, ν= 0.15
Contour=0.0005



Δρ3: ΔE= -6.74, ν= 0.18
Contour=0.0005



Δρ3: ΔE= -4.3, ν=0.17
Contour=0.0005

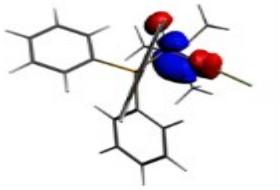


Δρ4: ΔE= -4.70, ν= 0.16
Contour=0.0003

Δρ rest: ΔE= -6.94

Δρ4: ΔE= -4.70, ν= 0.16
Contour=0.0003

Δρ rest: ΔE= -6.62

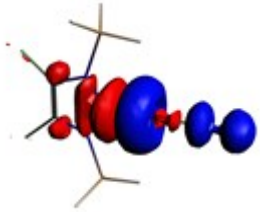


Δρ4: ΔE= -3.16, ν=0.14
Contour=0.0005

Δρ rest: ΔE= -9.57

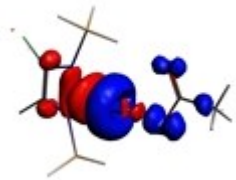
Fig. S7. Deformation densities associated with the most important orbital interactions for [NHC(Si(CH3)3)→CuR′] And [{P(Ph)$_3$CHSi(CH3)3}→CuCl](R′=Cl, OAc) complexes.

[NHC(SiH3)→CuCl]



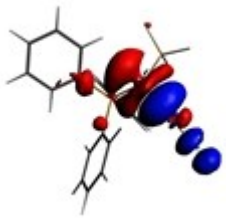
Δρ1: ΔE =-23.02, ν = 0.40
Contour =

[NHC(SiH3)→CuCl]

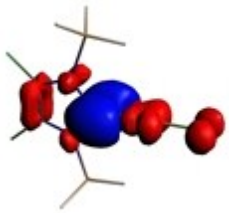


Δρ1: ΔE =-4.04, ν =0.42
Contour =0.001

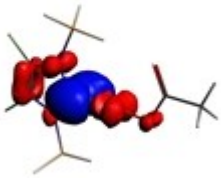
[{(Ph)$_3$PCH SiH3}→CuCl]



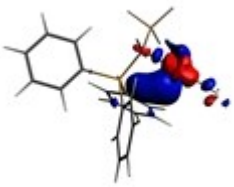
Δρ1: ΔE =-25.54, ν =0.47
Contour =0.001



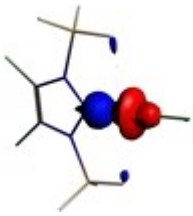
Δρ2: ΔE =-11.83, ν = 0.37
Contour =



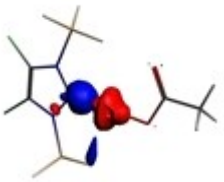
Δρ2: ΔE =-11.91, ν = 0.37
Contour =



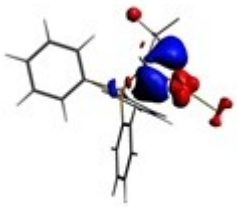
Δρ2: ΔE =-7.89, ν = 0.26
Contour =0.0005



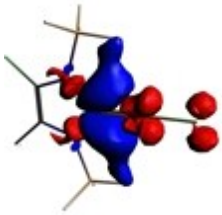
Δρ3: ΔE =-5.87, ν = 0.18
Contour =



Δρ3: ΔE =-6.83, ν = 0.19
Contour =

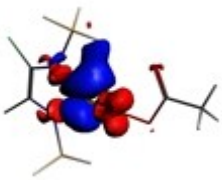


Δρ3: ΔE =-4.69, ν = 0.19
Contour =0.0005



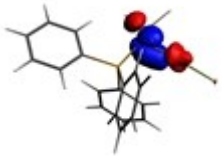
Δρ4: ΔE =-4.98, ν = 0.17
Contour =

Δρ rest: ΔE = -4.72



Δρ4: ΔE =-4.96, ν =0.16
Contour =

Δρ rest: ΔE = -4.3



Δρ4: ΔE =-3.93, ν =0.15
Contour =0.0005

Δρ rest: ΔE = -8.74

Fig. S8. Deformation densities associated with the most important orbital interactions for [NHC(SiH3)→CuR′] And [{P(Ph)$_3$CHSiH3}→CuCl](R′=Cl, OAc) complexes.

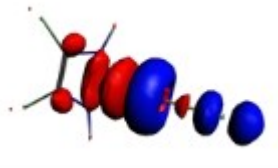
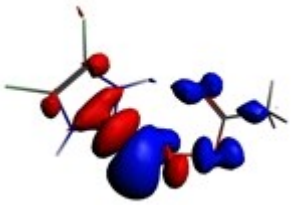
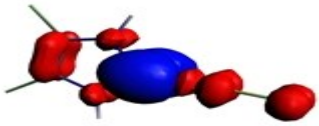
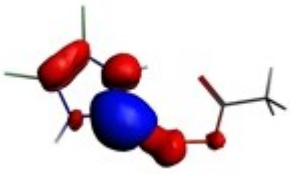
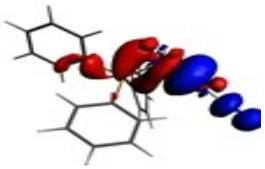
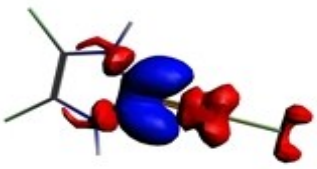
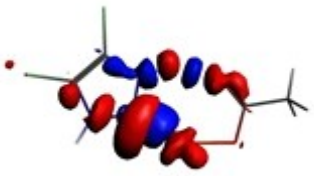
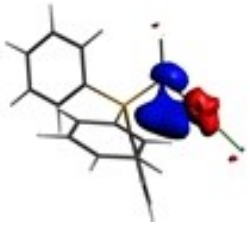
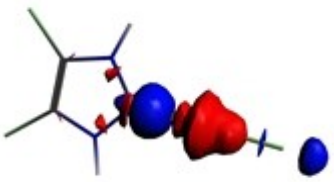
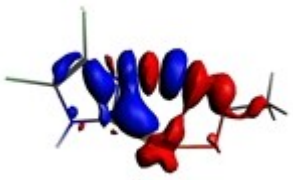
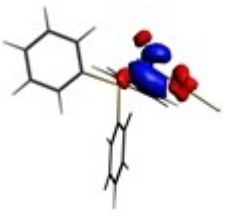
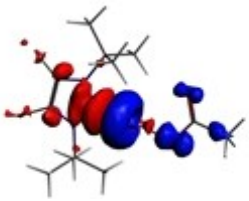
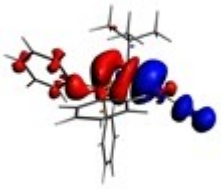
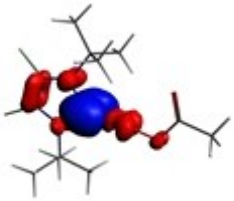
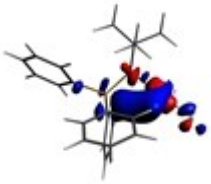
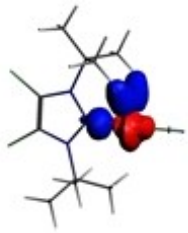
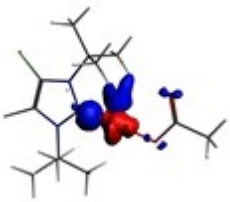
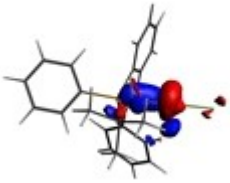
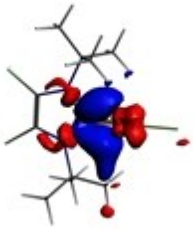
[NHC(H)→CuCl]	[NHC(H)→CuOAC]	[{(Ph)$_3$PCHH}→CuCl]
		
Δρ1: ΔE =-19.57, ν = 0.38 Contour =0.001	Δρ1: ΔE =-24.48, ν = 0.49 Contour =	Δρ1: ΔE =-27.67, ν = 0.49 Contour =0.001
		
Δρ2: ΔE =-11.23, ν = 0.37 Contour =0.0005	Δρ2: ΔE =-10.80, ν = 0.33 Contour =	Δρ2: ΔE =-8.03, ν = 0.26 Contour =0.001
		
Δρ3: ΔE =-4.76, ν = 0.17 Contour =0.0005	Δρ3: ΔE =-10.69, ν = 0.23 Contour =0.0005	Δρ3: ΔE =-3.34, ν = 0.15 Contour =0.0005
		
Δρ4: ΔE =-5.26, ν = 0.14 Contour =0.0003 Δρ rest: ΔE = -1.74	Δρ4: ΔE =-5.73, ν =0.18 Contour =0.0003 Δρ rest: ΔE = -3.69	Δρ4: ΔE =-3.43, ν = 0.15 Contour =0.0005 Δρ rest: ΔE = -7.38

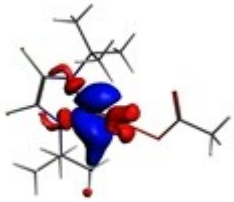
Fig. S9. Deformation densities associated with the most important orbital interactions for [NHC(H)→CuR′] And [{$P(Ph)_3$CHH}→CuCl](R′=Cl, OAc) complexes.

[NHC(C(CH3)3)→CuCl]	**[NHC(C(CH3)3)→CuOAC]**	**[{$(Ph)_3$PCHC(CH3)3}→CuCl]**
		
Δρ1: ΔE =-23.39, ν =0.40 Contour =0.001	Δρ1: ΔE =-24.41, ν = 0.42 Contour =0.001	Δρ1: ΔE =-28.31, ν = 0.52 Contour =0.001
		
Δρ2: ΔE =-10.33, ν = 0.33 Contour =0.0005	Δρ2: ΔE =-10.70, ν = 0.33 Contour =0.0005	Δρ2: ΔE =-8.83, ν = 0.29 Contour =0.001
		
Δρ3: ΔE =-6.72, ν = 0.18 Contour =0.0005	Δρ3: ΔE =-7.34, ν = 0.19 Contour =0.0005	Δρ3: ΔE =-4.05, ν = 0.17 Contour =0.0005



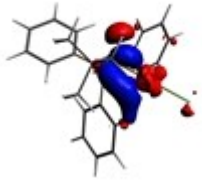
Δρ4: ΔE =-4.76, ν = 0.15
Contour =0.0003

Δρ rest: ΔE = -7.69



Δρ4: ΔE =-4.8, ν = 0.16
Contour =0.0003

Δρ rest: ΔE = -8.5

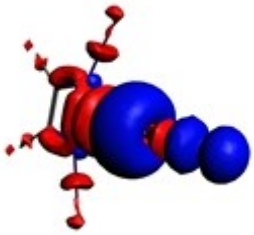


Δρ4: ΔE =-3.17, ν = 0.15
Contour =0.0003

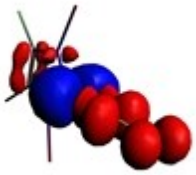
Δρ rest: ΔE = -7.8

Fig. S10. Deformation densities associated with the most important orbital interactions for [NHC(C(CH3)3)→CuR′] And [{P(Ph)$_3$CHC(CH3)3}→CuCl](R′=Cl, OAc) complexes.

[NHC(Br)→AuCl]

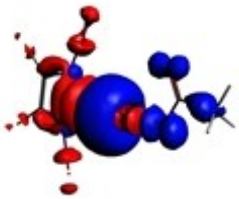


Δρ1: ΔE =-41.96, ν = 0.61
Contour =0.001

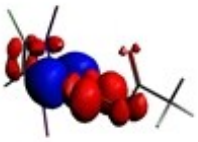


Δρ2: ΔE =-14.37, ν = 0.41
Contour =0.0005

[NHC(Br)→AuOAC]



Δρ1: ΔE =-44.75, ν = 0.65
Contour =0.001

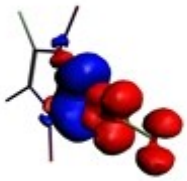


Δρ2: ΔE =-15.08, ν =0.41
Contour =0.0005

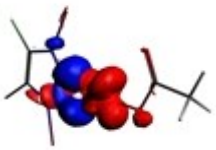
[{(Ph)$_3$PCHBr}→AuCl]

Δρ1: ΔE =-43.98, ν = 0.65
Contour =0.001

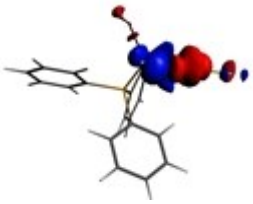
Δρ2: ΔE =-9.24, ν = 0.33
Contour =0.0005



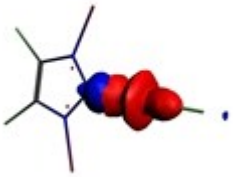
Δρ3: ΔE =-7.5, ν =0.23
Contour =0.0005



Δρ3: ΔE =-9.14, ν = 0.23
Contour =0.0005

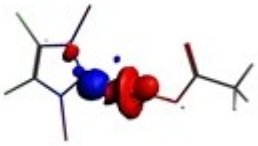


Δρ3: ΔE =-8.49, ν = 0.25
Contour =0.0005



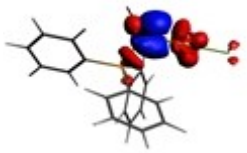
Δρ4: ΔE =-8.96, ν = 0.19
Contour =0.0007

Δρ rest: ΔE = -4.16



Δρ4: ΔE =-8.90, ν = 0.19
Contour =0.0008

Δρ rest: ΔE = -4.91



Δρ4: ΔE =-4.53, ν = 0.17
Contour =0.0005

Δρ rest: ΔE = -7.60

Fig. S11. Deformation densities associated with the most important orbital interactions for [NHC(Br)→AuR′] And [{$P(Ph)_3$CHCBr}→AuCl](R′=Cl, OAc) complexes.

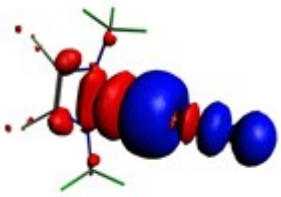
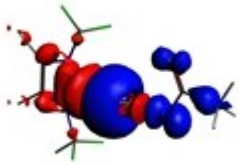
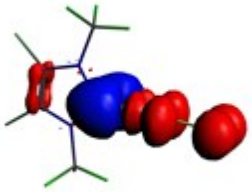
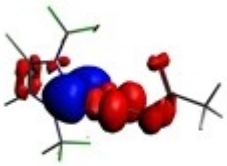
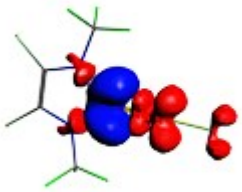
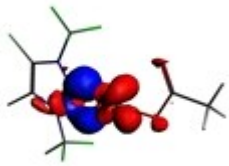
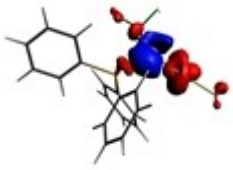
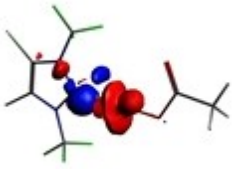
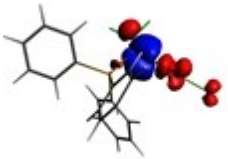
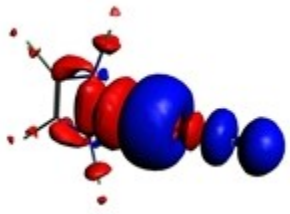
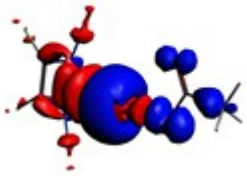
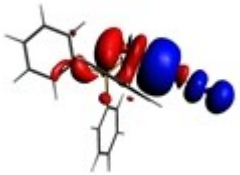
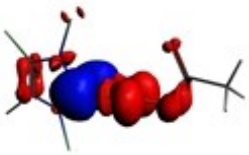
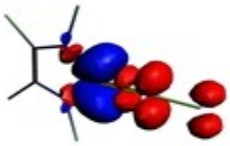
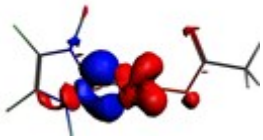
[NHC(CF3)→AuCl]	[NHC(CF3)→AuOAC]	[{(Ph)$_3$PCHCF3}→AuCl]
		
Δρ1: ΔE =-38.59, ν = 0.55 Contour =0.001	Δρ1: ΔE =-41.08, ν =0.58 Contour =0.001	Δρ1: ΔE =-40.200.61, ν = Contour =0.001
		
Δρ2: ΔE =-16.6, ν = 0.47 Contour =0.0005	Δρ2: ΔE =-17.38, ν = 0.47 Contour =0.0005	Δρ2: ΔE =-9.02, ν = 0.29 Contour =0.001
		
Δρ3: ΔE =-7.22, ν = 0.21 Contour =0.0005	Δρ3: ΔE =-9.11, ν = 0.22 Contour =0.0005	Δρ3: ΔE =-4.73, ν = 0.17 Contour =0.0005
		
Δρ4: ΔE =-8.23, ν = 0.18 Contour =0.0007	Δρ4: ΔE =-8.83, ν = 0.2 Contour =0.0007	Δρ4: ΔE =-3.98, ν = 0.16 Contour =0.0005
Δρ rest: ΔE = -3.67	Δρ rest: ΔE = -4.12	Δρ rest: ΔE = -7.81

Fig. S12. Deformation densities associated with the most important orbital interactions for [NHC(CF3)→AuR′] and [{$P(Ph)_3$CHCCF3}→AuCl](R′=Cl, OAc) complexes.

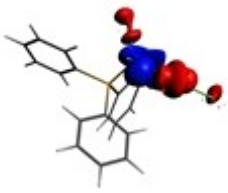
[NHC(Cl)→AuCl]	**[NHC(Cl)→AuOAC]**	**[{$(Ph)_3$PCHCl}→AuCl]**
		
Δρ1: ΔE =-40.76, ν = 0.58 Contour =0.001	Δρ1: ΔE =-43.24, ν =0.61 Contour =0.001	Δρ1: ΔE =-43.55, ν = 0.65 Contour =0.001
		
Δρ2: ΔE =-15.06, ν = 0.43 Contour =0.0005	Δρ2: ΔE =--15.80, ν = 0.43 Contour =0.0005	Δρ2: ΔE =-9.4, ν =0.31 Contour =0.001



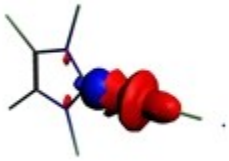
Δρ3: ΔE =-7.73, ν = 0.23
Contour =0.0005



Δρ3: ΔE =-9.30, ν = 0.22
Contour =0.0005

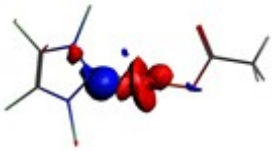


Δρ3: ΔE =-7.35, ν = 0.23
Contour =0.0005



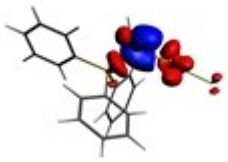
Δρ4: ΔE =-9.05, ν = 0.19
Contour =0.0007

Δρ rest: ΔE = -3.49



Δρ4: ΔE =-9.12, ν = 0.20
Contour =0.0007

Δρ rest: ΔE = -3.96



Δρ4: ΔE =-4.45, ν = 0.17
Contour =0.0005

Δρ rest: ΔE = -7.50

Fig. S13. Deformation densities associated with the most important orbital interactions for [NHC(Cl)→AuR′] And [{$P(Ph)_3$CHCCl}→AuCl](R′=Cl, OAc) complexes.

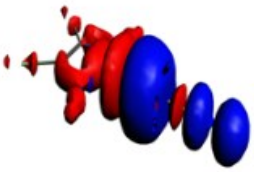
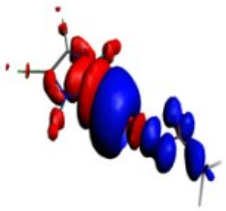
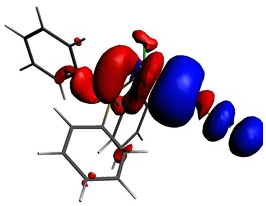
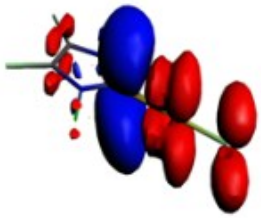
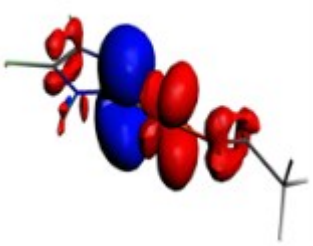
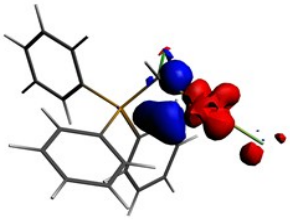
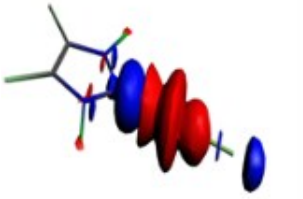
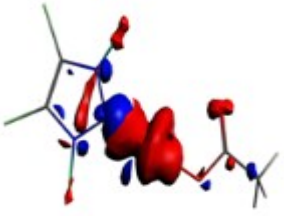
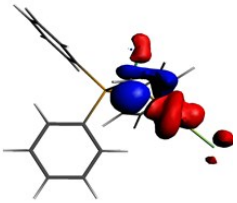
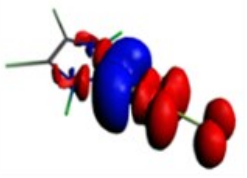
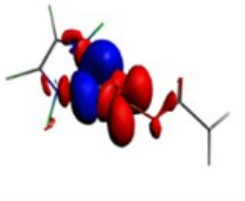
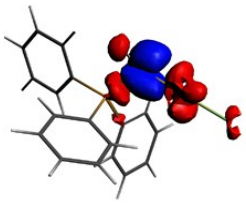
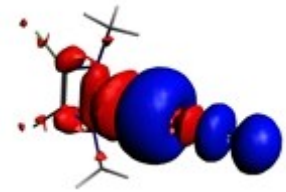
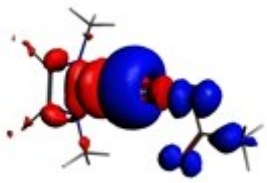
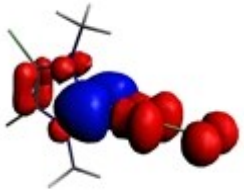
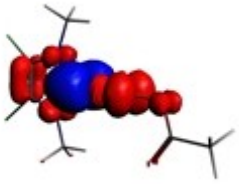
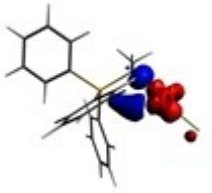
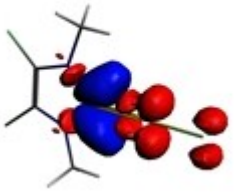
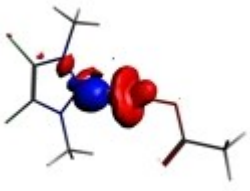
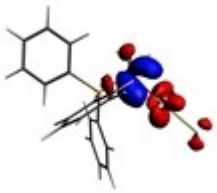
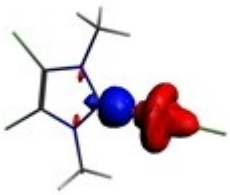
[NHC(F)→AuCl]	[NHC(F)→AuOAC]	[{(Ph)$_3$PCHF}→AuCl]
		
Δρ1: ΔE= -38.91, ν= 0.56 Contour=0.001	Δρ1: ΔE= -41.92, ν= 0.59 Contour=0.001	Δρ1: ΔE= -46.19, ν= 0.68 Contour=0.001
		
Δρ2: ΔE= -14.29, ν= 0.42 Contour=0.0005	Δρ2: ΔE= -15.39, ν= 0.4 Contour=0.0005	Δρ2: ΔE= -10.6, ν= 0.31 Contour=0.001
		
Δρ3: ΔE= -10.44, ν= 0.23 Contour=0.0005	Δρ3: ΔE= -13.1, ν= 0.28 Contour=0.0005	Δρ3: ΔE= -6.84, ν= 0.23 Contour=0.0005
		
Δρ4: ΔE= -7.70, ν= 0.22 Contour=0.0003	Δρ4: ΔE= -7.96, ν= 0.21 Contour=0.0003	Δρ4: ΔE= -4.62, ν= 0.18 Contour=0.0005
Δρ rest: ΔE= -2.48	Δρ rest: ΔE= -2.84	Δρ rest: ΔE= -7.07

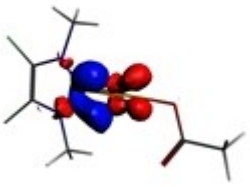
Fig. S14. Deformation densities associated with the most important orbital interactions for [NHC(F)→AuR′] And [{P(Ph)$_3$CHCF}→AuCl](R′=Cl, OAc) complexes.

[NHC(Me)→AuCl]	**[NHC(Me)→AuOAC]**	**[{(Ph)$_3$PCHCMe}→AuCl]**
		
Δρ1: ΔE =-41.52, ν = 0.57 Contour =0.001	Δρ1: ΔE =-44.69, ν =060 Contour =0.001	Δρ1: ΔE =-44.84, ν = 0.66 Contour =0.001
		
Δρ2: ΔE =-11.94, ν = -0.37 Contour =0.0005	Δρ2: ΔE =-12.55, ν = 0.36 Contour =0.0005	Δρ2: ΔE =-9.95, ν = 0.30 Contour =0.001
		
Δρ3: ΔE =-6.52, ν = 0.20 Contour =0.0005	Δρ3: ΔE =-10.52, ν = 0.2 Contour =0.0008	Δρ3: ΔE =-3.99, ν =0.16 Contour =0.0005



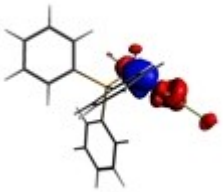
Δρ4: ΔE =-8.83, ν = 0.2
Contour =0.0007

Δρ rest: ΔE = -4.70



Δρ4: ΔE =-6.69, ν = 0.19
Contour =0.0008

Δρ rest: ΔE = -5.52



Δρ4: ΔE =-3.73, ν = 0.15
Contour =0.0005

Δρ rest: ΔE = -7.78

Fig. S15. Deformation densities associated with the most important orbital interactions for [NHC(CH3)→AuR′] And [{P(Ph)$_3$CHCCH3}→AuCl](R′=Cl, OAc) complexes.

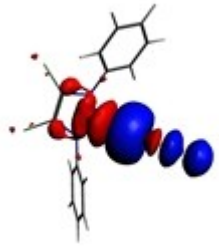
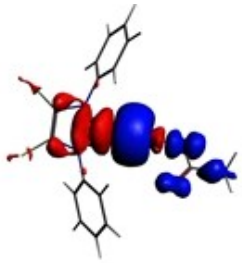
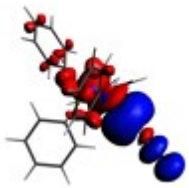
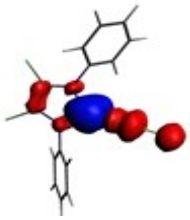
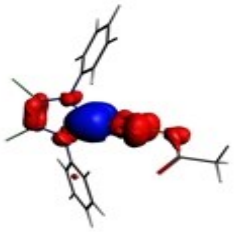
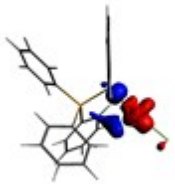
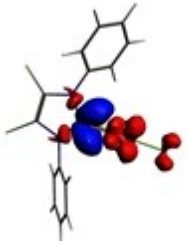
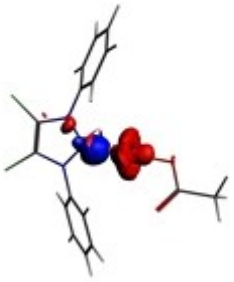
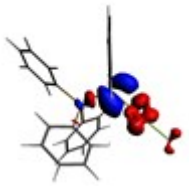
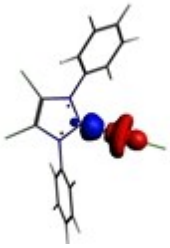
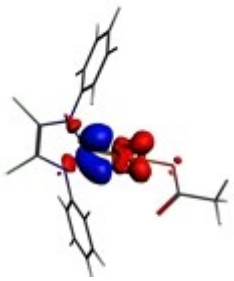
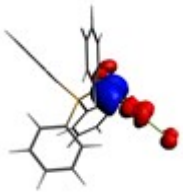
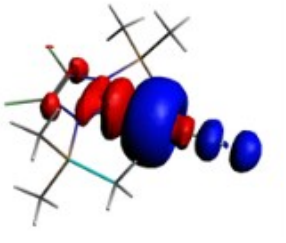
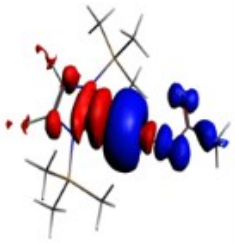
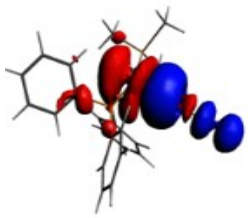
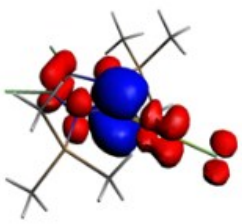
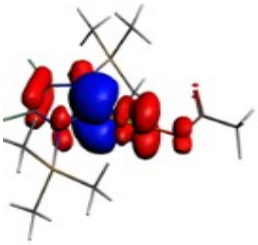
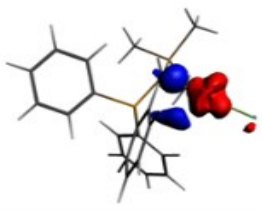
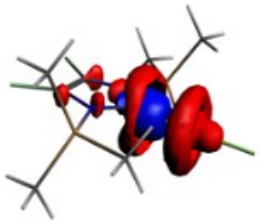
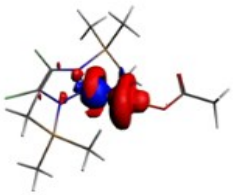
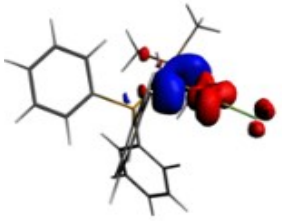
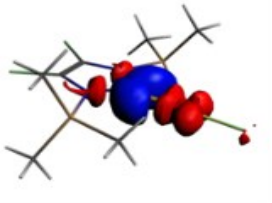
[NHC(Ph)→AuCl]	[NHC(Ph)→AuOAC]	[{(Ph)$_3$PCHPh}→AuCl]
		
Δρ1: ΔE =-41.12, ν = 0.57 Contour =0.001	Δρ1: ΔE =-44.29, ν = 0.61 Contour =0.001	Δρ1: ΔE =-45.06, ν = 0.69 Contour =0.001
		
Δρ2: ΔE =-13.43, ν =0.40 Contour =0.0005	Δρ2: ΔE =-14.12, ν = 0.38 Contour =0.0005	Δρ2: ΔE =-9.92, ν = 0.28 Contour =0.001
		
Δρ3: ΔE =-6.57, ν =0.20 Contour =0.0005	Δρ3: ΔE =-10.17, ν = 0.21 Contour =0.0007	Δρ3: ΔE =-4.06, ν = 0.17 Contour =0.0005
		
Δρ4: ΔE =-8.85, ν =0.20 Contour =0.0007	Δρ4: ΔE =-6.86, ν = 0.19 Contour =0.0007	Δρ4: ΔE =-0.3.74, ν = 0.16 Contour =0.0005
Δρ rest: ΔE = -4.92	Δρ rest: ΔE = -6.79	Δρ rest: ΔE = -6.80

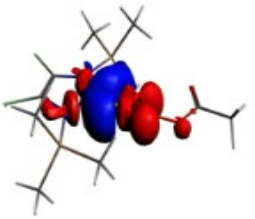
Fig. S16. Deformation densities associated with the most important orbital interactions for [NHC(Ph)→AuR′] And [{P(Ph)$_3$CHCPh}→AuCl](R′=Cl, OAc) complexes.

[NHC(Si(CH3)3)→AuCl]	**[NHC(Si(CH3)3)→AuOAC]**	**[{(Ph)$_3$PCH Si(CH3)3}→AuCl]**
		
Δρ1: ΔE= -22.78, ν= 0.44 Contour=0.001	Δρ1: ΔE= -46.53, ν= 0.62 Contour=0.001	Δρ1: ΔE= -42.07, ν= 0.63 Contour=0.001
		
Δρ2: ΔE= -9.72, ν= 0.30 Contour=0.000	Δρ2: ΔE= -11.83, ν= 0.35 Contour=0.000	Δρ2: ΔE= -8.9, ν= 0.27 Contour=0.001
		
Δρ3: ΔE= -9.98, ν= 0.21 Contour=0.0005	Δρ3: ΔE= -9.88, ν= 0.22 Contour=0.0005	Δρ3: ΔE= -4.5, ν= 0.18 Contour=0.0005



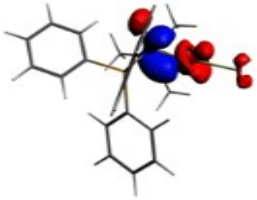
Δρ4: ΔE= -5.27, ν= 0.16
Contour=0.0003

Δρ rest: ΔE= -6.69



Δρ4: ΔE= -6.04, ν= 0.18
Contour=0.0003

Δρ rest: ΔE= -9.81

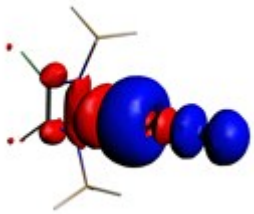


Δρ4: ΔE= -3.5, ν= 0.15
Contour=0.0005

Δρ rest: ΔE= -9.34

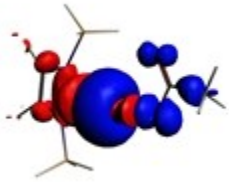
Fig. S17. Deformation densities associated with the most important orbital interactions for [NHC(Si(CH3)3)→AuR′] And [{P(Ph)$_3$CHCSi(CH3)3}→AuCl](R′=Cl, OAc) complexes.

[NHC(SiH3)→AuCl]



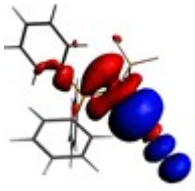
Δρ1: ΔE =-41.34, ν =057
Contour =0.001

[NHC(SiH3)→AuOAC]

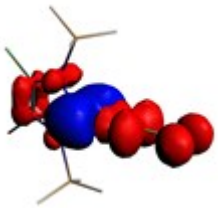


Δρ1: ΔE =-44.38, ν = 0.60
Contour =0.001

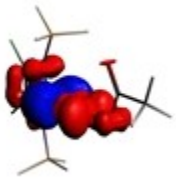
[{(Ph)$_3$PCHCSiH3}→AuCl]



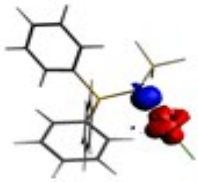
Δρ1: ΔE =-41.08, ν =0.63
Contour =0.001



Δρ2: ΔE =-13.04, ν = 01.
Contour =0.0005

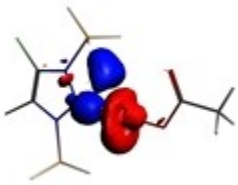


Δρ2: ΔE =-13.52, ν = 0.38
Contour =0.0005

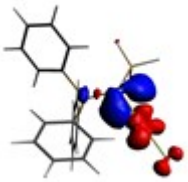


Δρ2: ΔE =-9.43, ν = 0.27
Contour =0.001

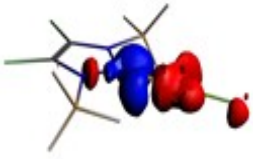
Δρ3: ΔE =-8.66, ν =0.24
Contour =0.0005



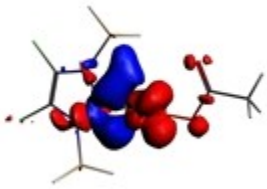
Δρ3: ΔE =-10.28, ν = 0.24
Contour =0.0005



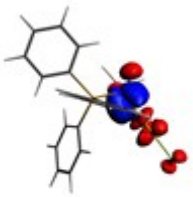
Δρ3: ΔE =-4.8, ν = 0.20
Contour =0.0005



Δρ4: ΔE =-7.59, ν = 0.20
Contour =0.0007



Δρ4: ΔE =-7.68, ν = 0.21
Contour =0.0003



Δρ4: ΔE =-3.93, ν = 0.20
Contour =0.005

Δρ rest: ΔE = -6.06

Δρ rest: ΔE = -5.19

Δρ rest: ΔE = -6.93

Fig. S18. Deformation densities associated with the most important orbital interactions for [NHC(SiH3)→AuR′] And [{$P(Ph)_3$CHCSiH3}→AuCl](R′=Cl, OAc) complexes.

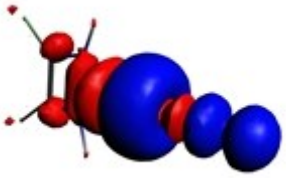
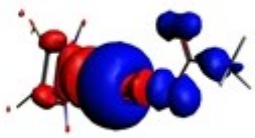
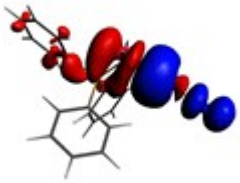
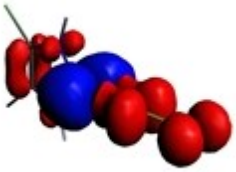
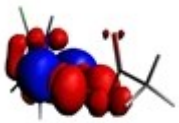
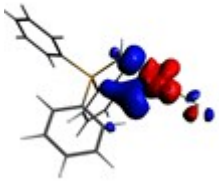
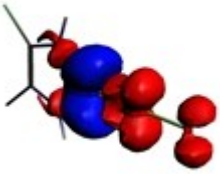
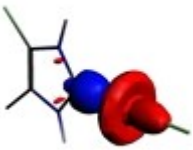
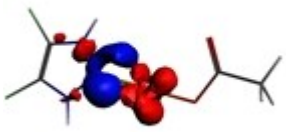
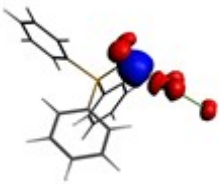
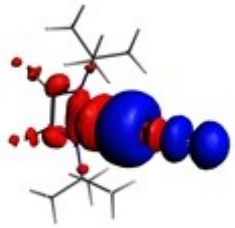
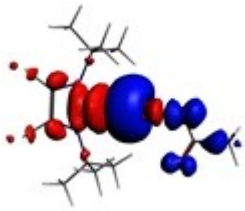
[NHC(H)→AuCl]	[NHC(H)→AuOAC]	[{(Ph)$_3$PCHH}→AuCl]
		
Δρ1: ΔE =-41.13, ν =0.56 Contour =0.001	Δρ1: ΔE =-43.68, ν = 0.59 Contour =0.001	Δρ1: ΔE =-45.14, ν = 0.66 Contour =0.001
		
Δρ2: ΔE =-13.35, ν = 0.40 Contour =0.0005	Δρ2: ΔE =-14.09, ν = 0.40 Contour =0.0005	Δρ2: ΔE =-9.87, ν = 0.28 Contour =0.001
		
Δρ3: ΔE =-6.57, ν = 0.20 Contour =0.0005	Δρ3: ΔE =-9.75, ν = 0.21 Contour =0.0007	Δρ3: ΔE =4.12, ν = 0.16 Contour =0.0005
		
Δρ4: ΔE =-8.65, ν = 0.19 Contour =0.0007	Δρ4: ΔE =-7.14, ν = 0.19 Contour =0.0007	Δρ4: ΔE =-3.72, ν = 0.16 Contour =0.0005
Δρ rest: ΔE = -2.98	Δρ rest: ΔE = -3.33	Δρ rest: ΔE = -7.43

Fig. S19. Deformation densities associated with the most important orbital interactions for [NHC(H)→AuR′] And [{P(Ph)$_3$CHH}→AuCl](R′=Cl, OAc) complexes.

[NHC(C(CH3)3)→AuCl] **[NHC(C(CH3)3)→AuOAC]** **[{(Ph)$_3$PCHC(CH3)3}→AuCl]**

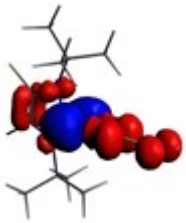


Δρ1: ΔE =-40.84, ν =0.57
Contour =0.001

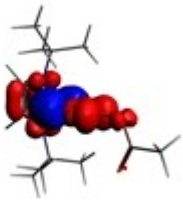


Δρ1: ΔE =-44.17, ν = 0.61
Contour =0.001

Δρ1: ΔE =-43.97, ν = 0.65
Contour =0.001

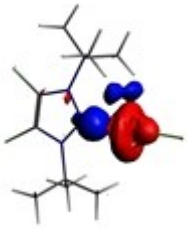


Δρ2: ΔE =-10.95, ν = 0.34
Contour =0.0005

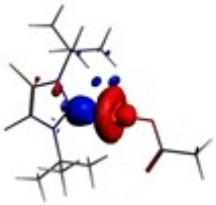


Δρ2: ΔE =-11.50, ν = 0.34
Contour =0.0005

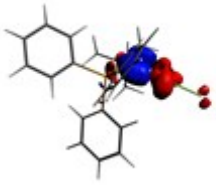
Δρ1: ΔE =-9.91, ν = 0.30
Contour =0.001



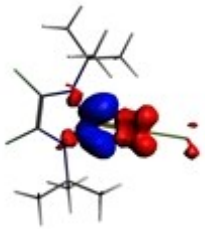
Δρ3: ΔE =--8.7, ν = 0.21
Contour =0.0005



Δρ3: ΔE =-10.58, ν = 0.22
Contour =0.0005



Δρ2: ΔE =-4.18, ν = 0.16
Contour =0.0005

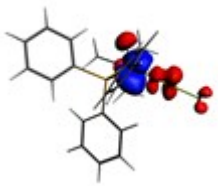


Δρ4: ΔE =-5.74, ν = 0.18
Contour =0.0007

Δρ rest: ΔE = -6.05

Δρ4: ΔE =,-5.89 ν = 0.17
Contour =0.0007

Δρ rest: ΔE = -10.19

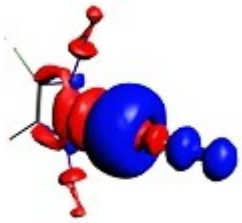


Δρ3: ΔE =-3.68, ν = 0.16
Contour =0.0005

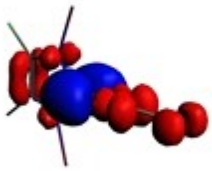
Δρ rest: ΔE = -9.76

Fig. S20. Deformation densities associated with the most important orbital interactions for [NHC(C(CH3)3)→AuR′] And [{P(Ph)$_3$CHCC(CH3)3}→AuCl](R′=Cl, OAc) complexes.

[NHC(Br)→AgCl]

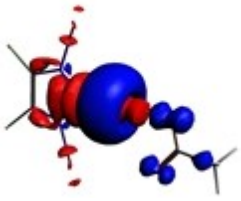


Δρ1: ΔE =-18.78, ν = 0.45
Contour =0.001

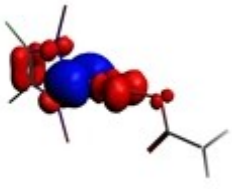


Δρ2: ΔE =-8.30, ν = 0.30
Contour =0.0005

[NHC(Br)→AgOAC]

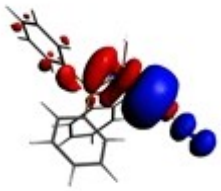


Δρ1: ΔE =-18.89, ν =0.45
Contour =0.001

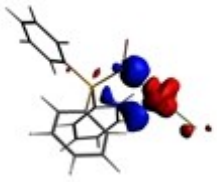


Δρ2: ΔE =-8.15, ν =0.31
Contour =0.0005

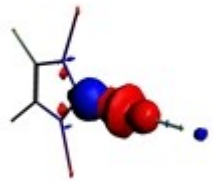
[{(Ph)$_3$PCHBr}→AgCl]



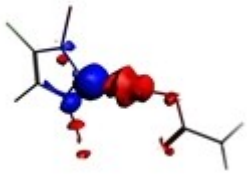
Δρ1: ΔE =-24.04, ν = 0.51
Contour =0.001



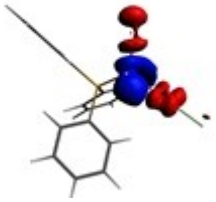
Δρ2: ΔE =-7.15, ν =0.24
Contour =0.0005



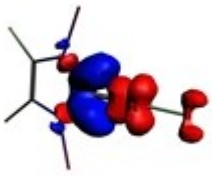
Δρ3: ΔE =-7.0, ν = 0.18
Contour =0.0005



Δρ3: ΔE =-8.32, ν = 0.28
Contour =0.0007

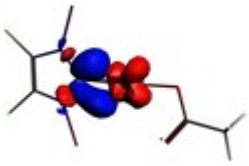


Δρ3: ΔE =-3.51, ν = 0.16
Contour =0.0005



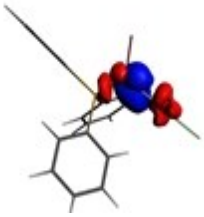
Δρ4: ΔE =-4.35, ν = 0.17
Contour =0.0005

Δρ rest: ΔE = -3.7



Δρ4: ΔE =-4.56, ν = 0.16
Contour =

Δρ rest: ΔE = -2.64



Δρ4: ΔE =-2.35, ν = 0.11
Contour =0.0005

Δρ rest: ΔE = -7.95

Fig. S21. Deformation densities associated with the most important orbital interactions for [NHC(Br)→AgR′] And [{P(Ph)$_3$CHCBr}→AgCl](R′=Cl, OAc) complexes.

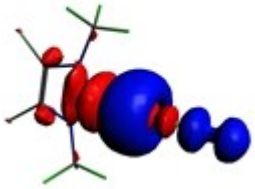
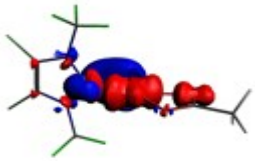
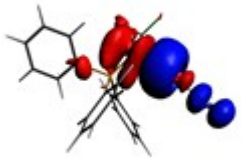
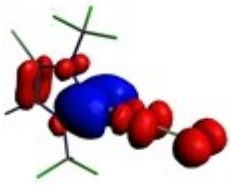
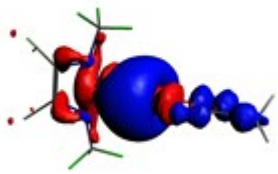
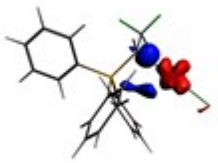
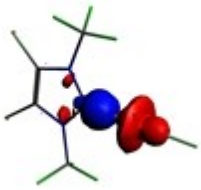
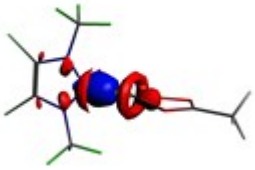
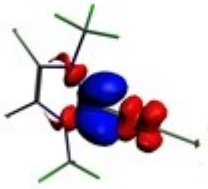
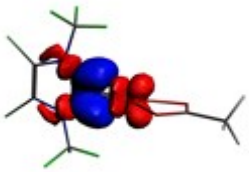
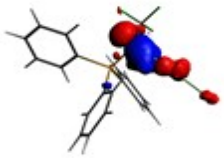
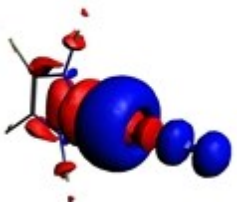
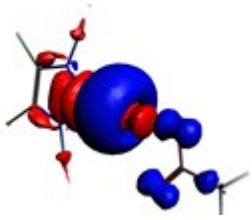
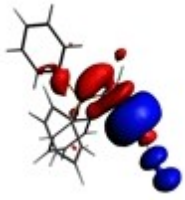
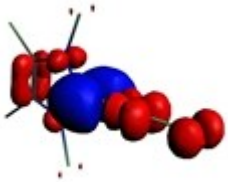
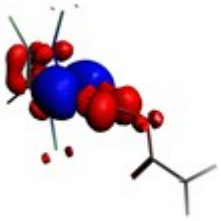
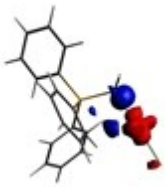
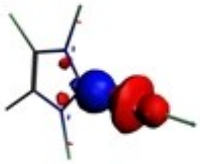
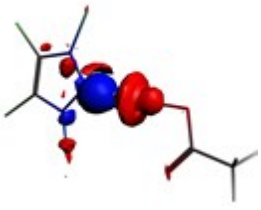
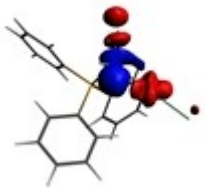
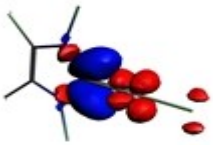
[NHC(CF3)→AgCl]	[NHC(CF3)→AgOAC]	[{(Ph)$_3$PCHCF3}→AgCl]
		
Δρ1: ΔE =-16.25, ν = 0.39 Contour =0.001	Δρ1: ΔE =-13.71, ν =0.45 Contour =0.0008	Δρ1: ΔE =-21.34, ν = 0.45 Contour =0.001
		
Δρ2: ΔE =-9.19, ν = 0.36 Contour =0.0005	Δρ2: ΔE =-18.76, ν = 0.42 Contour =0.0005	Δρ2: ΔE =-6.13, ν = 0.23 Contour =0.001
		
Δρ3: ΔE =--6.14, ν = 0.17 Contour =0.0005	Δρ3: ΔE =-7.23, ν = 0.18 Contour =0.0007	Δρ3: ΔE =-2.69, ν = 0.12 Contour =0.0003
		
Δρ4: ΔE =-4.10, ν = 0.15 Contour =0.0005	Δρ4: ΔE =-3.8, ν =0.14 Contour =0.0003	Δρ4: ΔE =-2.06, ν = 0.11 Contour =0.0003
Δρ rest: ΔE = -3.11	Δρ rest: ΔE = -2.33	Δρ rest: ΔE = -6.01

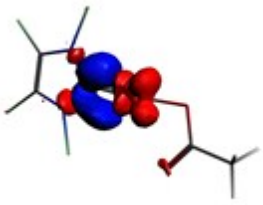
Fig. S22. Deformation densities associated with the most important orbital interactions for [NHC(CF3)→AgR′] And [{P(Ph)$_3$CHCCF3}→AgCl](R′=Cl, OAc) complexes.

[NHC(Cl)→AgCl]	**[NHC(Cl)→AgOAC]**	**[{(Ph)$_3$PCHCl}→AgCl]**
		
Δρ1: ΔE =-17.95, ν = 0.4 Contour =0.001	Δρ1: ΔE =-22.25, ν = 0.46 Contour =0.001	Δρ1: ΔE =-23.38, ν =0.49 Contour =0.001
		
Δρ2: ΔE =-8.68, ν = 0.32 Contour =0.0005	Δρ2: ΔE =-8.42, ν = 0.30 Contour =0.0005	Δρ2: ΔE =-7.12, ν = 0.25 Contour =0.001
		
Δρ3: ΔE =-6.90, ν = 0.18 Contour =0.0005	Δρ3: ΔE =-8.11, ν = 0.21 Contour =0.0007	Δρ3: ΔE =-3.97, ν = 0.17 Contour =0.0005



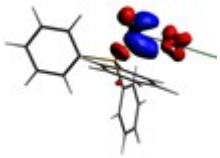
Δρ4: ΔE =-4.14, ν = 0.17
Contour =0.0005

Δρ rest: ΔE = -2.76



Δρ4: ΔE =-4.39, ν = 0.16
Contour =0.0005

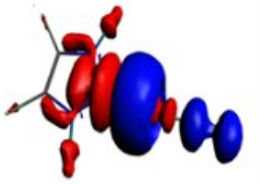
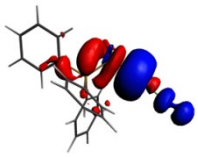
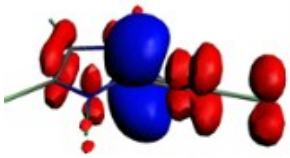
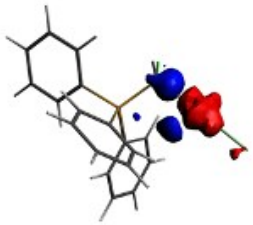
Δρ rest: ΔE = -2.29

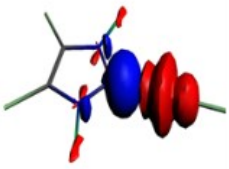


Δρ4: ΔE =-2.46, ν = 0.011
Contour =0.0005

Δρ rest: ΔE = -5.73

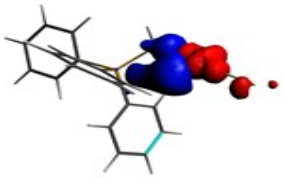
Fig. S23. Deformation densities associated with the most important orbital interactions for [NHC(Cl)→AgR′] And [{P(Ph)$_3$CHCCl}→AgCl](R′=Cl, OAc) complexes.

[NHC(F)→AgCl]	**[NHC(F)→AgOAC]**	**[{(Ph)$_3$PCHF}→AgCl]**
		
Δρ1: ΔE= -20.50, ν= 0.41 Contour=0.001	-	Δρ1: ΔE= -25.12, ν= 0.52 Contour=0.001
	-	
Δρ2: ΔE= -7.97, ν= 0.30 Contour=0.0005		Δρ2: ΔE= -7.78, ν= 0.26 Contour=0.001

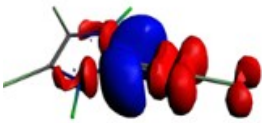


Δρ3: ΔE= -8.10, ν= 0.22
Contour=0.0005

-

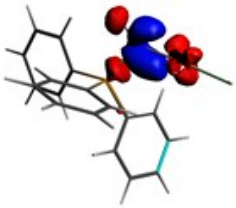


Δρ3: ΔE= -3.69, ν= 0.17
Contour=0.0005



Δρ4: ΔE= -4.0, ν= 0.15
Contour=0.0003

-



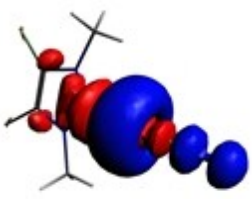
Δρ4: ΔE= -2.58, ν= 0.12
Contour=0.0005

Δρ rest: ΔE= -1.52

Δρ rest: ΔE= -5.30

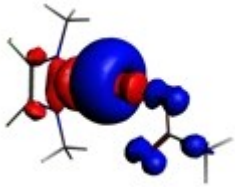
Fig. S24. Deformation densities associated with the most important orbital interactions for [NHC(F)→AgR′] And [{P(Ph)$_3$CHCF}→AgCl](R′=Cl, OAc) complexes.

[NHC(Me)→AgCl]



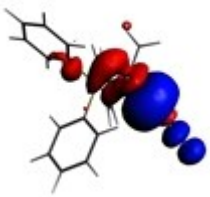
Δρ1: ΔE =-18.46, ν = 0.41
Contour =0.001

[NHC(Me)→AgCl]

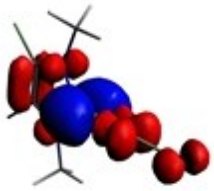


Δρ1: ΔE =-20.68, ν =0.45
Contour =0.001

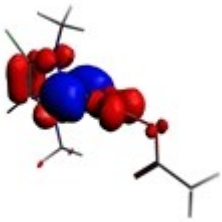
[{(Ph)$_3$PCHMe}→AgCl]



Δρ1: ΔE =-24.43, ν =0.51
Contour =0.001

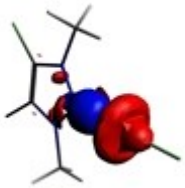


Δρ2: ΔE =-7.12, ν = 0.27
Contour =0.0005

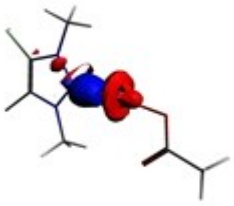


Δρ2: ΔE =-7.31, ν = 0.26
Contour =0.0005

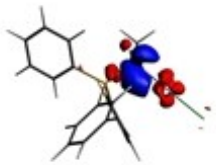
Δρ2: ΔE =-7.33, ν = 0.25
Contour =0.001



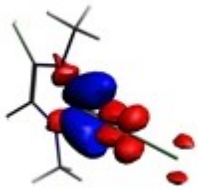
Δρ3: ΔE =-6.48, ν = 0.17
Contour =0.0005



Δρ3: ΔE =-7.91, ν = 0.20
Contour =0.001

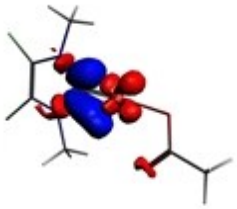


Δρ3: ΔE =-2.39, ν = 0.12
Contour =0.0005



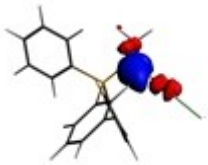
Δρ4: ΔE =-3.94, ν = 0.15
Contour =0.0005

Δρ rest: ΔE = -3.57



Δρ4: ΔE =-4.03, ν = 0.14
Contour =0.0005

Δρ rest: ΔE = -4.29

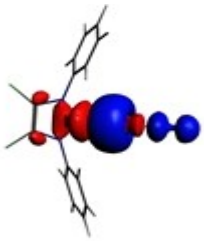


Δρ4: ΔE =-2.21, ν = 0.11
Contour =0.0005

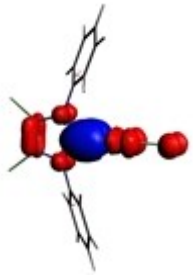
Δρ rest: ΔE = -5.99

Fig. S25. Deformation densities associated with the most important orbital interactions for [NHC(CH3)→AgR′] And [{$P(Ph)_3$CHCCH3}→AgCl](R′=Cl, OAc) complexes.

[NHC(Ph)→AgCl]

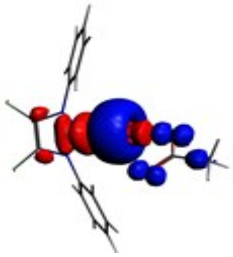


Δρ1: ΔE =-18.20, ν = 0.41
Contour=0.001

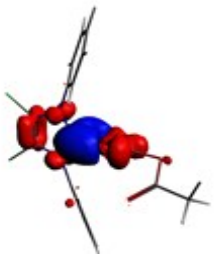


Δρ2: ΔE =-7.90, ν = 0.9
Contour =0.0005

[NHC(Ph)→AgCl]



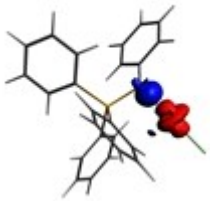
Δρ1: ΔE =-19.92, ν = 0.45
Contour =0.001



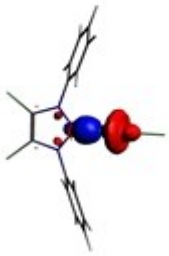
Δρ2: ΔE =-8.40, ν =0.28
Contour =0.0005

[{$(Ph)_3$PCHPh}→AgCl]

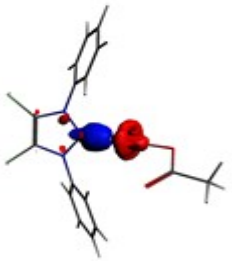
Δρ1: ΔE =-23.8, ν = 0.50
Contour =0.001



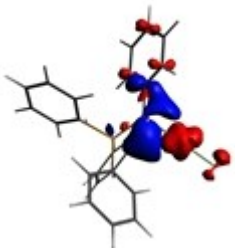
Δρ2: ΔE =-7.00, ν = 0.23
Contour =0.001



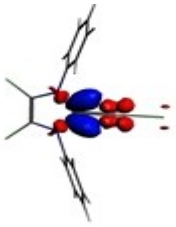
Δρ3: ΔE =-6.45, ν = 0.18
Contour =0.0005



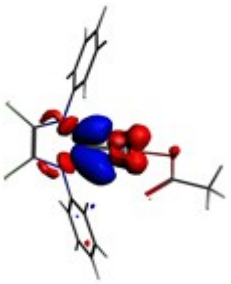
Δρ3: ΔE =-7.34, ν = 0.19
Contour =0.0008



Δρ3: ΔE =-2.62, ν =0.14
Contour =0.0003



Δρ4: ΔE =-3.88, ν = 0.15
Contour =0.0005



Δρ4: ΔE =-4.00, ν = 0.14
Contour =0.0003

NO DATA

Δρ rest: ΔE = -4.40

Δρ rest: ΔE = -5.68

Δρ rest: ΔE = -8.57

Fig. S26. Deformation densities associated with the most important orbital interactions for [NHC(Ph)→AgR′] And [{$P(Ph)_3$CHCPh}→AgCl](R′=Cl, OAc) complexes.

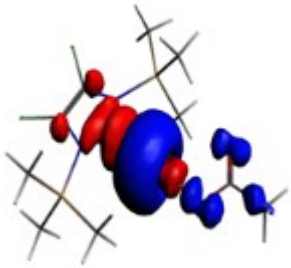
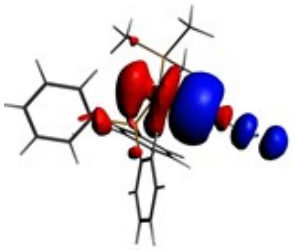
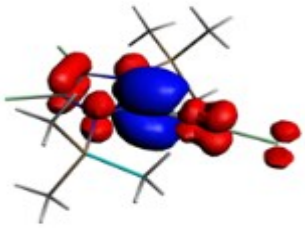
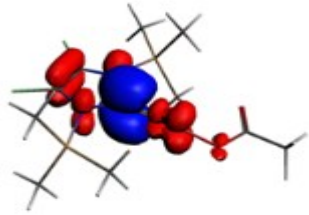
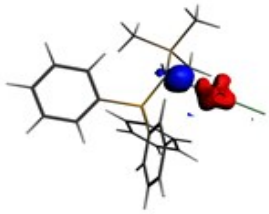
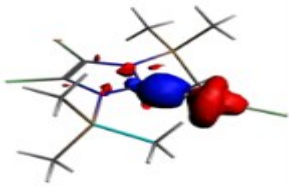
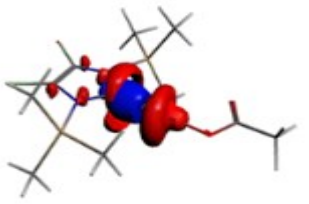
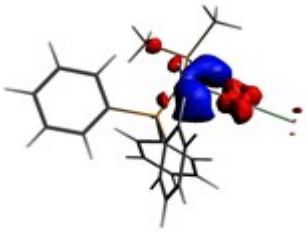
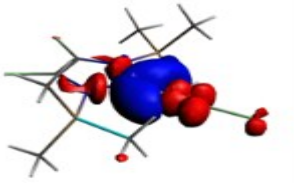
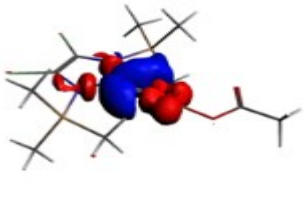
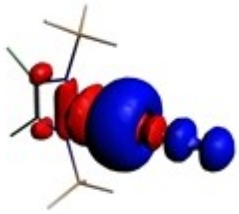
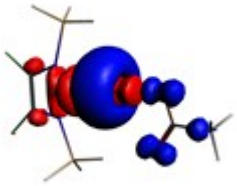
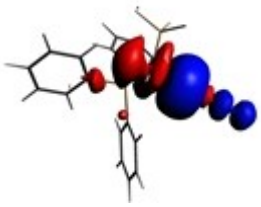
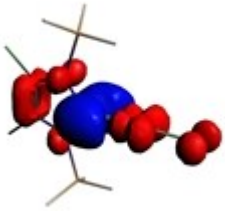
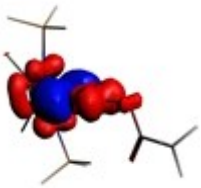
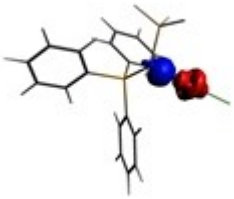
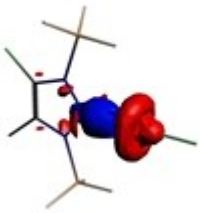
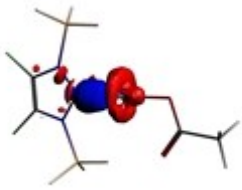
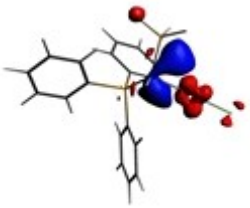
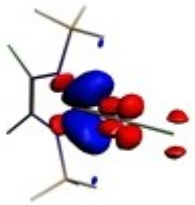
[NHC(Si(CH3)3)→AgCl]	[NHC(Si(CH3)3)→AgOAC]	[{(Ph)$_3$PCHSi(CH3)3}→AgCl]
		
Δρ1: ΔE= -23.22, ν=0. 44 Contour=0.001	Δρ1: ΔE= -25.12, ν=0. 48 Contour=0.001	Δρ1: ΔE= -22.76, ν= 0.48 Contour=0.001
		
ρ2: ΔE= -6.5, ν= 0.25 Contour=0.0005	Δρ2: ΔE= -6.7, ν= 0.25 Contour=0.0005	Δρ2: ΔE= -6.67, ν= 0.23 Contour=0.001
		
Δρ3: ΔE= -6.37, ν= 0.18 Contour=0.0005	Δρ3: ΔE= -7.3, ν= 0.19 Contour=0.0005	Δρ3: ΔE= -2.9, ν= 0.13 Contour=0.0005
		
Δρ4: ΔE= -3.45, ν= 0.14 Contour=0.0003	Δρ4: ΔE= -3.5, ν= 0.13 Contour=0.0003	Δρ4: ΔE= -2.1, ν= 0.11 Contour=0.0005
Δρ rest: ΔE= -6.59	Δρ rest: ΔE= -7.95	Δρ rest: ΔE= -7.27

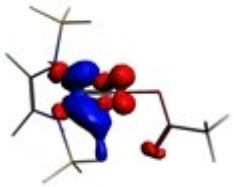
Fig. S27. Deformation densities associated with the most important orbital interactions for [NHC(Si(CH3)3)→AgR′] And [{P(Ph)$_3$CHCSi(CH3)3}→AgCl](R′=Cl, OAc) complexes.

[NHC(SiH3)→AgCl]	**[NHC(SiH3)→AgCl]**	**[{(Ph)$_3$PCHSiH3}→AgCl]**
		
Δρ1: ΔE =-18.18, ν = 0.41 Contour =0.001	Δρ1: ΔE =-20.17, ν =0.45 Contour =0.001	Δρ1: ΔE =-21.92, ν = 0.47 Contour =0.001
		
Δρ2: ΔE =-7.71, ν = 0.9 Contour =0.0005	Δρ2: ΔE =-7.93, ν = 0.28 Contour =0.0005	Δρ2: ΔE =-6.83, ν = 0.23 Contour =0.001
		
Δρ3: ΔE =-6.43, ν = 0.18 Contour =0.0005	Δρ3: ΔE =-7.65, ν = 0.20 Contour =0.0008	Δρ3: ΔE =-3.14, ν = 0.15 Contour =0.0005



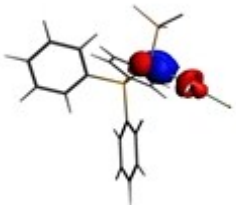
Δρ4: ΔE =-4.01, ν = 0.15
Contour =0.0005

Δρ rest: ΔE = -4.64



Δρ4: ΔE =-4.05, ν = 0.15
Contour =0.0005

Δρ rest: ΔE = -5.98



Δρ4: ΔE =-2.23, ν = 0.11
Contour =0.0005

Δρ rest: ΔE = -6.62

Fig. S28. Deformation densities associated with the most important orbital interactions for [NHC(SiH3)→AgR′] And [{$P(Ph)_3$CHCSiH3}→AgCl](R′=Cl, OAc) complexes.

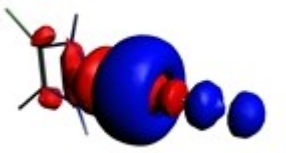
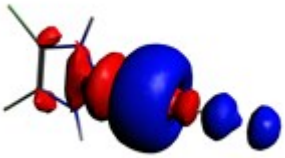
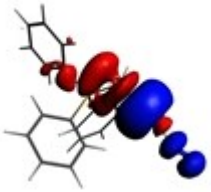
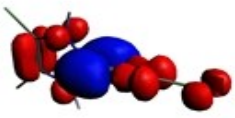
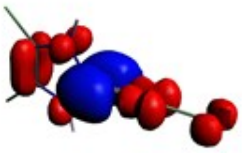
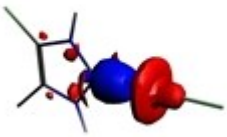
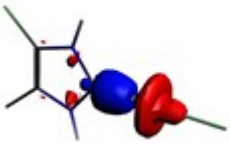
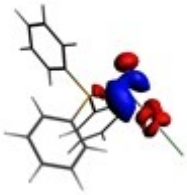
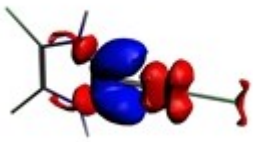
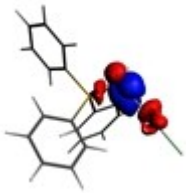
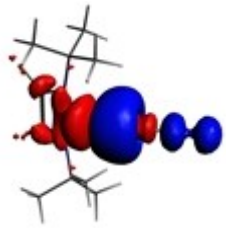
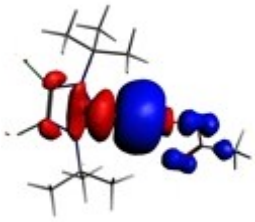
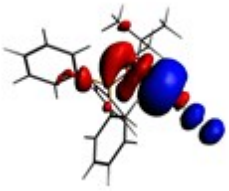
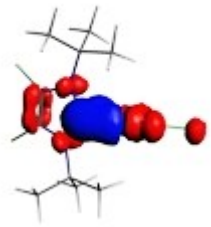
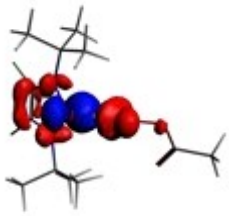
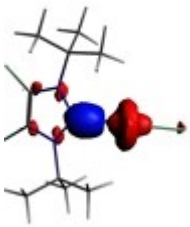
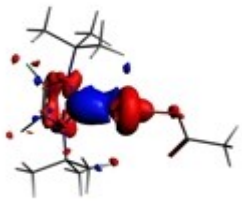
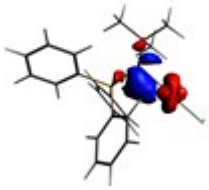
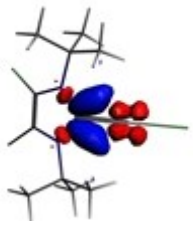
[NHC(H)→AgCl]	[NHC(H)→AgCl]	[{(Ph)$_3$PCHH}→AgCl]
		
Δρ1: ΔE =-14.83, ν =0.37 Contour =0.001	Δρ1: ΔE =-14.83, ν = 0.37 Contour =0.001	Δρ1: ΔE =-24.39, ν = 0.49 Contour =0.001
		
Δρ2: ΔE =-7.30, ν = 0.27 Contour =0.0005	Δρ2: ΔE =-7.30, ν = 0.27 Contour =0.0005	Δρ2: ΔE =-7.55, ν = 0.24 Contour =0.001
		
Δρ3: ΔE =-6.31, ν =0.16 Contour =0.0005	ρΔ3: ΔE =-6.31, ν = 0.16 Contour =0.0008	ρΔ3: ΔE =-2.33, ν = 0.12 Contour =0.0005
		
Δρ4: ΔE =-3.70, ν = 0.14 Contour =0.0005	Δρ4: ΔE =-3.70, ν = 0.14 Contour =0.0005	Δρ4: ΔE =-2.26, ν = 0.11 Contour =0.0005
Δρ rest: ΔE = -2.19	Δρ rest: ΔE = -2.195	Δρ rest: ΔE = -5.4

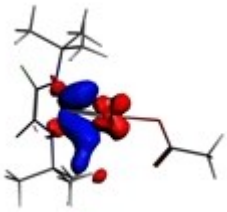
Fig. S29. Deformation densities associated with the most important orbital interactions for [NHC(H)→AgR′] And [{$P(Ph)_3CHH$}→AgCl](R′=Cl, OAc) complexes.

[NHC(C(CH3)3)→AgCl]	**[NHC(C(CH3)3)→AgCl]**	**[{$(Ph)_3PCHC(CH3)3$}→AgCl]**
		
Δρ1: ΔE =-18.02, ν =0.41 Contour =0.001	Δρ1: ΔE =-23.00, ν =0.46 Contour =0.001	Δρ1: ΔE =-23.86, ν =0.49 Contour =0.001
		
Δρ2: ΔE =-8.04, ν= 0.26 Contour =0.0005	Δρ2: ΔE =-9.44, ν =0.27 Contour =0.0003	Δρ2: ΔE =-7.01, ν =0.5 Contour =0.001
		
Δρ3: ΔE =-4.86, ν = 0.16 Contour =0.0005	Δρ3: ΔE =-4.67, ν = 0.16 Contour =0.0003	Δρ3: ΔE =-2.46, ν =0.12 Contour =0.0005



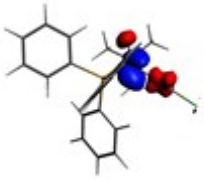
Δρ4: ΔE =-3.38, ν =0.13
Contour =0.0005

Δρ rest: ΔE = -5.18



Δρ4: ΔE =-3.32, ν = 0.13
Contour =0.0005

Δρ rest: ΔE = -6.23



Δρ4: ΔE =-2.10, ν =0.11
Contour =0.0005

Δρ rest: ΔE = -7.65

Fig. S 30. Deformation densities associated with the most important orbital interactions for [NHC(C(CH3)3)→AgR′] And [{$P(Ph)_3$CHCC(CH3)3}→AgCl](R′=Cl, OAc) complexes.

Optimized Coordinates of the studied complexeshere at PBE/def2-TZVP for

All (complex 1-120)

[NHC(SiH3)→CuOAc]

E= -3013.566154

C	-0.080523000	14.589805000	6.305249000
C	0.651103000	14.886915000	8.428564000
N	0.837420000	15.243404000	7.096563000
Cu	-0.249366000	14.725836000	4.456282000
C	-0.390342000	14.004576000	8.474287000
N	-0.837725000	13.823938000	7.168318000
Cl	1.602356000	15.493907000	9.700867000
Cl	-1.085492000	13.219515000	9.814455000
Si	-2.192353000	12.770782000	6.621253000
H	-1.870563000	11.373321000	7.023169000
H	-3.432851000	13.239713000	7.298960000
H	-2.232232000	12.955221000	5.147920000
Si	2.077917000	16.385470000	6.424283000

H	3.408535000	15.827373000	6.798498000
H	1.809181000	16.409536000	4.961260000
H	1.861888000	17.690228000	7.111525000
O	-0.491217000	14.787537000	2.601963000
C	0.313309000	15.663735000	2.052025000
O	1.129571000	16.360978000	2.675499000
C	0.173468000	15.770609000	0.542514000
H	-0.862572000	16.029648000	0.281318000
H	0.386081000	14.795912000	0.080063000
H	0.858328000	16.526931000	0.144581000

[NHC(Ph)→CuOAc]

E= -3475.218921

C	0.077325000	14.485183000	6.371914000
C	0.403604000	15.168670000	8.520275000
N	0.847692000	15.263432000	7.202166000
Cu	0.159403000	14.405089000	4.512903000
C	-0.658372000	14.304890000	8.521273000
N	-0.845555000	13.896045000	7.202467000
Cl	1.037505000	16.038041000	9.834195000
Cl	-1.567009000	13.757692000	9.847283000
C	1.955655000	16.049136000	6.732196000
C	3.197555000	15.944067000	7.366104000
C	1.782636000	16.867520000	5.612935000
C	4.275232000	16.683786000	6.878972000
C	2.875362000	17.587021000	5.126075000
C	4.116599000	17.505140000	5.759796000
H	3.325446000	15.277339000	8.218820000

H	0.821931000	16.923868000	5.096161000
H	5.246878000	16.602397000	7.368578000
H	2.741315000	18.209371000	4.240517000
H	4.965282000	18.074293000	5.376856000
C	-1.836287000	12.970218000	6.736102000
C	-1.423799000	11.858339000	5.996842000
C	-3.190074000	13.200556000	6.992143000
C	-2.381240000	10.970516000	5.506396000
C	-4.137977000	12.299537000	6.505290000
C	-3.736990000	11.186841000	5.762467000
H	-0.361598000	11.701747000	5.807641000
H	-3.498908000	14.085234000	7.549237000
H	-2.062874000	10.105867000	4.922601000
H	-5.196805000	12.478937000	6.697187000
H	-4.483379000	10.490053000	5.378153000
O	0.200468000	14.310027000	2.636993000
C	0.143870000	15.517542000	2.136911000
O	0.069082000	16.558395000	2.813274000
C	0.177099000	15.565715000	0.617927000
H	-0.643856000	14.961126000	0.206770000
H	1.114969000	15.122058000	0.253332000
H	0.093697000	16.598402000	0.262588000

[NHC(H)→CuOAc]

E= -3013.566154

C	-0.643027000	14.056216000	5.991841000
C	0.661324000	15.122178000	7.518728000
N	0.381102000	14.937849000	6.181612000

Cu	-0.972874000	13.850090000	4.174492000
C	-0.218056000	14.327376000	8.211590000
N	-0.997617000	13.692244000	7.254990000
Cl	1.876852000	16.152855000	8.102005000
Cl	-0.408130000	14.088199000	9.882604000
H	-1.741068000	13.037126000	7.469717000
H	0.823816000	15.359826000	5.334890000
O	-0.557482000	14.290339000	2.380900000
C	0.425202000	15.141706000	2.439546000
O	0.961197000	15.560158000	3.496143000
C	0.921005000	15.633549000	1.093791000
H	0.095870000	16.115853000	0.550676000
H	1.247757000	14.778319000	0.485374000
H	1.748014000	16.340204000	1.218346000

[NHC(Si(CH3)3)→CuOAc]

E= -3830.412738

C	0.063365000	14.506576000	6.259376000
C	0.557361000	14.943885000	8.412808000
N	0.924670000	15.189313000	7.094321000
Cu	-0.103628000	14.730234000	4.414222000
C	-0.506405000	14.088564000	8.399782000
N	-0.808853000	13.805531000	7.071478000
Cl	1.281590000	15.649606000	9.787743000
Cl	-1.356288000	13.489205000	9.754129000
Si	-2.143035000	12.675798000	6.491511000
Si	2.337375000	16.244387000	6.531293000
O	-0.478672000	14.919224000	2.579941000

C	-0.273288000	16.136752000	2.147247000
O	0.149025000	17.073169000	2.845939000
C	-0.590482000	16.334987000	0.673100000
H	-1.622934000	16.021071000	0.463718000
H	0.067725000	15.697050000	0.065189000
H	-0.452779000	17.383211000	0.386742000
C	-1.833747000	11.011524000	7.301976000
H	-1.912469000	11.036869000	8.395820000
H	-2.575743000	10.290376000	6.925116000
H	-0.836978000	10.629601000	7.035848000
C	-3.766584000	13.454792000	7.010893000
H	-4.603227000	12.823599000	6.673784000
H	-3.847740000	13.570709000	8.099912000
H	-3.887023000	14.445024000	6.547598000
C	-2.066625000	12.463251000	4.637887000
H	-1.097828000	12.071794000	4.297567000
H	-2.837503000	11.716758000	4.377060000
H	-2.281523000	13.378072000	4.068187000
C	3.845880000	15.707286000	7.515482000
H	3.803518000	15.970885000	8.578871000
H	4.004085000	14.621595000	7.433733000
H	4.728357000	16.200540000	7.078418000
C	2.656305000	15.946833000	4.721692000
H	3.588707000	16.482952000	4.472196000
H	2.815325000	14.883517000	4.492343000
H	1.859262000	16.348594000	4.072285000
C	1.826689000	18.012515000	6.870283000
H	0.955915000	18.275805000	6.252129000

H	1.576371000	18.181626000	7.926798000
H	2.646424000	18.696079000	6.601231000

[NHC(F)→CuOAc]

E= -3443.50516

C	-0.154173000	-0.000941000	0.017024000
C	-2.374310000	-0.688897000	-0.026392000
N	-1.036648000	-1.035053000	0.068281000
Cu	1.684210000	-0.001244000	-0.089046000
C	-2.373454000	0.689811000	-0.026412000
N	-1.035392000	1.034321000	0.068276000
Cl	-3.656866000	-1.784723000	0.060076000
Cl	-3.654664000	1.787203000	0.059758000
F	-0.619452000	2.326359000	-0.146622000
F	-0.622331000	-2.327623000	-0.146581000
O	3.473235000	-0.000573000	-1.054161000
C	4.066000000	0.000018000	0.082207000
O	3.384343000	-0.000345000	1.158257000
C	5.573667000	0.001667000	0.127204000
H	5.953644000	0.890239000	-0.396411000
H	5.956687000	-0.877169000	-0.410270000
H	5.936907000	-0.005251000	1.160191000

[NHC(Br)→CuOAc]

E= -8159.823328

C	-0.096404000	14.553553000	6.160484000
C	0.556069000	15.067476000	8.313824000

N	0.732222000	15.306004000	6.954090000
Cu	-0.193851000	14.545374000	4.310059000
C	-0.431698000	14.117996000	8.403861000
N	-0.801101000	13.832559000	7.091376000
Cl	1.419514000	15.833016000	9.546710000
Cl	-1.109315000	13.402009000	9.775429000
O	-0.419028000	14.449454000	2.437024000
C	0.528108000	15.209915000	1.949706000
O	1.351233000	15.820357000	2.655998000
C	0.557406000	15.299970000	0.434979000
H	-0.402026000	15.691135000	0.067182000
H	0.679817000	14.295445000	0.005240000
H	1.375015000	15.948654000	0.103126000
Br	-2.104598000	12.604714000	6.613418000
Br	1.952679000	16.504190000	6.240676000

[NHC(Cl)→CuOAc]

E= -3932.321816

C	-0.098252000	14.534540000	6.147878000
C	0.565081000	15.068239000	8.300550000
N	0.738746000	15.285078000	6.935010000
Cu	-0.196935000	14.513307000	4.300802000
C	-0.432635000	14.131789000	8.404297000
N	-0.805550000	13.835832000	7.093481000
Cl	1.445235000	15.842600000	9.513954000
Cl	-1.119524000	13.435189000	9.779688000
Cl	1.867321000	16.364574000	6.289148000
Cl	-2.013348000	12.723120000	6.694168000

O	-0.414916000	14.400139000	2.423367000
C	0.507674000	15.204784000	1.962264000
O	1.288155000	15.840956000	2.695668000
C	0.567117000	15.314424000	0.450464000
H	-0.402311000	15.661024000	0.064732000
H	0.749344000	14.322083000	0.013551000
H	1.358681000	16.006406000	0.144022000

[NHC(CH3)→CuOAc]

E= -3092.101573

C	-0.129067000	14.431977000	6.221031000
C	0.550062000	15.097062000	8.281184000
N	0.754127000	15.215321000	6.916267000
Cu	-0.186295000	14.307221000	4.364846000
C	-0.487476000	14.217807000	8.452707000
N	-0.887458000	13.823697000	7.185749000
C	1.769421000	16.055607000	6.288371000
H	2.769895000	15.743540000	6.616409000
H	1.680842000	15.939716000	5.197670000
H	1.610586000	17.106230000	6.565720000
C	-1.966366000	12.890346000	6.904087000
H	-2.028302000	12.793044000	5.813743000
H	-1.755259000	11.910755000	7.353579000
H	-2.917966000	13.271552000	7.298221000
Cl	1.462268000	15.924869000	9.450731000
Cl	-1.207311000	13.662340000	9.888459000
O	-0.187832000	14.228656000	2.479918000
C	0.766663000	15.032290000	2.093482000

O	1.489415000	15.683944000	2.873788000
C	0.948680000	15.127390000	0.589518000
H	0.013514000	15.469143000	0.123229000
H	1.166079000	14.131138000	0.178384000
H	1.761954000	15.817536000	0.341416000

[NHC(CF3)→CuOAc]

E= -3687.287758

C	-0.027545000	-0.000743000	-0.003392000
C	-2.247189000	-0.678138000	0.000946000
N	-0.899954000	-1.078651000	-0.001881000
Cu	1.817424000	-0.002526000	-0.002546000
C	-2.245609000	0.681885000	0.000947000
N	-0.897440000	1.079269000	-0.001929000
Cl	-3.583599000	-1.717375000	0.003943000
Cl	-3.579649000	1.724164000	0.004162000
C	-0.487881000	2.470246000	-0.002796000
F	0.839513000	2.575953000	-0.007579000
F	-0.978328000	3.096529000	-1.091517000
F	-0.970487000	3.095779000	1.089834000
C	-0.493581000	-2.470582000	-0.002662000
F	-0.978140000	-3.095032000	1.089733000
F	-0.985020000	-3.095664000	-1.091626000
F	0.833546000	-2.579319000	-0.006856000
O	3.568756000	-0.003894000	-1.098580000
C	4.204305000	-0.002992000	0.010380000

O	3.561990000	-0.002998000	1.114249000
C	5.712799000	0.001603000	0.004903000
H	6.072118000	0.910038000	-0.499223000
H	6.080966000	-0.855753000	-0.575557000
H	6.111077000	-0.037508000	1.024304000

[NHC(C(CH3)3)→CuOAc]

E= -3327.706709

C	0.001479000	14.590111000	6.419434000
C	0.569570000	14.844379000	8.589662000
N	0.893797000	15.189492000	7.282538000
Cu	0.014172000	14.747295000	4.546133000
C	-0.528841000	14.027169000	8.536435000
N	-0.874334000	13.873939000	7.198519000
Cl	1.321763000	15.291075000	10.057598000
Cl	-1.294255000	13.347130000	9.905432000
C	-2.037303000	13.043256000	6.701313000
C	2.018520000	16.073404000	6.744685000
C	-1.811344000	11.580177000	7.120989000
H	-2.636150000	10.966763000	6.732772000
H	-0.873973000	11.201640000	6.689570000
H	-1.775919000	11.448761000	8.207845000
C	-3.339188000	13.623075000	7.281554000
H	-4.189858000	13.044226000	6.896083000
H	-3.372998000	13.584293000	8.375689000
H	-3.465715000	14.667058000	6.961914000
C	-2.144388000	13.083043000	5.175954000
H	-1.256812000	12.667876000	4.677018000

H	-3.006557000	12.460272000	4.894734000
H	-2.325297000	14.096381000	4.789281000
C	2.902559000	16.646980000	7.856295000
H	2.352411000	17.300459000	8.544220000
H	3.421739000	15.870770000	8.431525000
H	3.667740000	17.258475000	7.359257000
C	2.897515000	15.215585000	5.823435000
H	3.731103000	15.828876000	5.454972000
H	3.307743000	14.352756000	6.368145000
H	2.346792000	14.866132000	4.938199000
C	1.379958000	17.244002000	5.983639000
H	2.175829000	17.908006000	5.619687000
H	0.822791000	16.903976000	5.098765000
H	0.713153000	17.819830000	6.641855000
O	-0.095058000	14.812726000	2.677318000
C	0.828641000	15.549202000	2.108447000
O	1.716095000	16.165978000	2.714809000
C	0.727709000	15.593961000	0.590896000
H	-0.252684000	15.993988000	0.294280000
H	0.794587000	14.575490000	0.181919000
H	1.524642000	16.216284000	0.169864000

[NHC(SiH3)→CuCl]

E= -3826.408876

C	-0.026817000	14.562636000	6.471848000
C	0.629398000	14.827649000	8.627625000
N	0.875484000	15.189187000	7.305773000

Cl	-0.255590000	14.862403000	2.519308000
Cu	-0.134999000	14.704396000	4.610511000
C	-0.432647000	13.969434000	8.624003000
N	-0.832438000	13.809420000	7.299919000
Cl	1.544853000	15.406532000	9.939349000
Cl	-1.195984000	13.191378000	9.930002000
Si	-2.187854000	12.789780000	6.684118000
H	-1.908164000	11.383990000	7.087869000
H	-3.441005000	13.280294000	7.321712000
H	-2.159524000	12.994318000	5.213285000
Si	2.159257000	16.302825000	6.699373000
H	3.473071000	15.736139000	7.111986000
H	1.963334000	16.318184000	5.227167000
H	1.936360000	17.630435000	7.335998000

[NHC(Si(CH3)3)→CuCl]

E= -4062.137932

C	0.000030000	0.246496000	-0.044079000
C	0.682070000	-1.902046000	0.021205000
N	1.109176000	-0.578368000	-0.024733000
Cu	0.000028000	2.120767000	0.006907000
C	-0.682181000	-1.901996000	0.021236000
N	-1.109187000	-0.578279000	-0.024681000
Cl	1.702741000	-3.269584000	0.084405000
Cl	-1.702939000	-3.269474000	0.084349000
Si	-2.871182000	-0.028962000	-0.051438000
Si	2.871212000	-0.029133000	-0.051455000
C	-3.661367000	-0.835056000	-1.550388000

H	-3.667763000	-1.931137000	-1.504335000
H	-4.704939000	-0.492445000	-1.628795000
H	-3.143694000	-0.529581000	-2.471738000
C	-3.619113000	-0.594483000	1.571941000
H	-4.677040000	-0.292752000	1.613304000
H	-3.572738000	-1.683289000	1.705383000
H	-3.103606000	-0.119112000	2.419390000
C	-2.987333000	1.823809000	-0.218747000
H	-2.521083000	2.205841000	-1.137401000
H	-4.064506000	2.062723000	-0.268395000
H	-2.560224000	2.380403000	0.626735000
C	3.661574000	-0.835777000	-1.550011000
H	3.668363000	-1.931829000	-1.503418000
H	3.143745000	-0.530930000	-2.471483000
H	4.705016000	-0.492823000	-1.628643000
C	2.987404000	1.823573000	-0.219389000
H	4.064593000	2.062660000	-0.267803000
H	2.522178000	2.205199000	-1.138721000
H	2.559206000	2.380412000	0.625398000
C	3.618856000	-0.594027000	1.572265000
H	3.104568000	-0.116641000	2.419323000
H	3.570557000	-1.682580000	1.707104000
H	4.677360000	-0.294208000	1.612800000
Cl	0.000153000	4.234630000	0.140258000

[NHC(Ph)→CuCl]

E= -3706.943839

C	0.000000000	14.527000000	6.486764000
C	0.524293000	14.966700000	8.662252000
N	0.835404000	15.223453000	7.327806000
Cl	0.000000000	14.527000000	2.514213000
Cu	0.000000000	14.527000000	4.616353000
C	-0.524293000	14.087300000	8.662252000
N	-0.835404000	13.830547000	7.327806000
Cl	1.288574000	15.685801000	9.997165000
Cl	-1.288574000	13.368199000	9.997165000
C	1.870622000	16.095919000	6.853402000
C	3.185825000	15.920972000	7.291207000
C	1.548193000	17.087122000	5.922809000
C	4.185521000	16.758905000	6.796483000
C	2.558979000	17.909894000	5.425342000
C	3.875137000	17.751497000	5.864174000
H	3.427396000	15.126049000	7.996865000
H	0.516645000	17.199697000	5.587862000
H	5.214857000	16.622538000	7.131117000
H	2.312018000	18.676768000	4.690242000
H	4.662325000	18.397886000	5.473303000
C	-1.870622000	12.958081000	6.853402000
C	-1.548193000	11.966878000	5.922809000
C	-3.185825000	13.133028000	7.291207000
C	-2.558979000	11.144106000	5.425342000
C	-4.185521000	12.295095000	6.796483000
C	-3.875137000	11.302503000	5.864174000
H	-0.516645000	11.854303000	5.587862000
H	-3.427396000	13.927951000	7.996865000

H	-2.312018000	10.377232000	4.690242000
H	-5.214857000	12.431462000	7.131117000
H	-4.662325000	10.656114000	5.473303000

[NHC(F)→CuCl]

E= -3443.50516

C	0.000000000	14.527000000	6.413263000
C	0.543812000	14.952933000	8.636539000
N	0.811399000	15.161857000	7.295327000
Cl	0.000000000	14.527000000	2.464673000
Cu	0.000000000	14.527000000	4.556882000
C	-0.543812000	14.101067000	8.636539000
N	-0.811399000	13.892143000	7.295327000
Cl	1.410936000	15.631924000	9.911537000
Cl	-1.410936000	13.422076000	9.911537000
F	-1.832400000	13.093176000	6.886684000
F	1.832400000	15.960824000	6.886684000

[NHC(Cl)→CuCl]

E= -4164.048093

C	0.000000000	14.527000000	6.416978000
C	0.540078000	14.950124000	8.629882000
N	0.835821000	15.181178000	7.286688000
Cl	0.000000000	14.527000000	2.465765000
Cu	0.000000000	14.527000000	4.559160000
C	-0.540078000	14.103876000	8.629882000
N	-0.835821000	13.872822000	7.286688000
Cl	1.389257000	15.615242000	9.926879000

Cl	-1.389257000	13.438758000	9.926879000
Cl	2.100231000	16.171015000	6.761098000
Cl	-2.100231000	12.882985000	6.761098000

[NHC(CH3)→CuCl]

E= -3323.825028

C	0.019853000	14.501835000	6.440201000
C	0.478501000	15.026817000	8.603256000
N	0.836859000	15.215165000	7.277889000
Cl	0.158008000	14.325516000	2.477157000
Cu	0.085337000	14.418290000	4.571237000
C	-0.592574000	14.172175000	8.603798000
N	-0.856773000	13.864238000	7.278670000
C	1.934151000	16.056045000	6.822737000
H	2.887252000	15.698870000	7.234890000
H	1.957053000	15.993586000	5.727984000
H	1.772715000	17.097391000	7.131617000
C	-1.921316000	12.981828000	6.824351000
H	-1.866478000	12.945616000	5.729552000
H	-1.785042000	11.973073000	7.236299000
H	-2.900287000	13.371105000	7.134112000
Cl	1.275339000	15.759008000	9.912593000
Cl	-1.482599000	13.558444000	9.913945000

[NHC(CF3)→CuCl]

E= -3919.009913

C	-0.030778000	14.564163000	6.376795000
C	0.608156000	14.860337000	8.579785000

N	0.845987000	15.192542000	7.236533000
Cl	-0.230439000	14.805783000	2.432284000
Cu	-0.124837000	14.677947000	4.519087000
C	-0.446485000	13.998210000	8.580438000
N	-0.820368000	13.830442000	7.237545000
Cl	1.480536000	15.437210000	9.908649000
Cl	-1.184110000	13.258472000	9.910241000
C	-1.925260000	12.969265000	6.830116000
F	-2.076311000	12.981493000	5.511138000
F	-1.688126000	11.707578000	7.235261000
F	-3.064973000	13.392162000	7.408560000
C	1.909405000	16.103868000	6.827804000
F	1.721751000	17.305390000	7.405205000
F	3.098969000	15.621032000	7.232883000
F	1.926882000	16.253104000	5.508667000

[NHC(C(CH3)3)→CuCl]

E= -3559.432858

C	0.010700000	14.547232000	6.501500000
C	0.544347000	14.851935000	8.675985000
N	0.893326000	15.161754000	7.365696000
Cl	0.230414000	14.867919000	2.516624000
Cu	0.077471000	14.672322000	4.615213000
C	-0.559397000	14.042094000	8.622497000
N	-0.882549000	13.858414000	7.282787000
Cl	1.274159000	15.331159000	10.144957000
Cl	-1.355462000	13.402156000	9.993082000
C	-2.042723000	13.024664000	6.781225000

C	2.033641000	16.020482000	6.826925000
C	-1.836978000	11.570645000	7.239749000
H	-2.660584000	10.956132000	6.851292000
H	-0.896158000	11.173058000	6.833837000
H	-1.822673000	11.464872000	8.329966000
C	-3.350687000	13.627636000	7.321979000
H	-4.197218000	13.044364000	6.934657000
H	-3.405679000	13.615972000	8.415974000
H	-3.464738000	14.663780000	6.973571000
C	-2.112833000	13.034054000	5.253960000
H	-1.216909000	12.602759000	4.784469000
H	-2.972305000	12.412990000	4.961242000
H	-2.275368000	14.040490000	4.841905000
C	2.904857000	16.616907000	7.937073000
H	2.348169000	17.291971000	8.598137000
H	3.406200000	15.851577000	8.541675000
H	3.684428000	17.208981000	7.438600000
C	2.923001000	15.132609000	5.943724000
H	3.754139000	15.734859000	5.551223000
H	3.341345000	14.297679000	6.524104000
H	2.369184000	14.724596000	5.084078000
C	1.421003000	17.177663000	6.023793000
H	2.229689000	17.811069000	5.633417000
H	0.834837000	16.815218000	5.165143000
H	0.771349000	17.794996000	6.660785000

[NHC(Br)→CuCl]

E= -8391.549527

C	0.305090000	-0.000323000	-0.000049000
C	-1.900988000	-0.685517000	0.000169000
N	-0.560733000	-1.064605000	-0.000004000
Cu	2.166266000	-0.001003000	0.000125000
C	-1.900235000	0.687349000	0.000179000
N	-0.559556000	1.064968000	0.000011000
Cl	-3.206403000	-1.756439000	0.000334000
Cl	-3.204473000	1.759700000	0.000366000
Br	0.037998000	2.819078000	-0.000372000
Br	0.034858000	-2.819388000	-0.000361000
Cl	4.260707000	-0.001593000	0.000487000

[NHC(H)→CuCl]

E= -3245.288908

C	0.000000000	14.527000000	6.437919000
C	0.539140000	14.948907000	8.626246000
N	0.839787000	15.184028000	7.293472000
Cl	0.000000000	14.527000000	2.481116000
Cu	0.000000000	14.527000000	4.576349000
C	-0.539140000	14.105093000	8.626246000
N	-0.839787000	13.869972000	7.293472000
Cl	1.404890000	15.626374000	9.916748000
Cl	-1.404890000	13.427626000	9.916748000
H	-1.598721000	13.276018000	6.975954000
H	1.598721000	15.777982000	6.975954000

[NHC(Cl)→AuOAc]

E= -2427.80732

Cl	6.271608000	6.118574000	3.909191000
Cl	5.653929000	7.680108000	7.012429000
N	5.962609000	4.061485000	5.678444000
N	5.589531000	5.006235000	7.552257000
C	5.715052000	3.759409000	6.993514000
C	5.751041000	6.040851000	6.630519000
C	5.991065000	5.434233000	5.424887000
Cl	6.206866000	2.886969000	4.491788000
Cl	5.271345000	5.246458000	9.192097000
Au	5.569555000	2.030443000	7.891258000
O	5.429300000	0.210850000	8.770628000
C	5.180418000	0.238536000	10.072460000
O	5.036939000	1.257365000	10.745947000
C	5.085943000	-1.156084000	10.669081000
H	6.021849000	-1.704694000	10.491768000
H	4.283107000	-1.721247000	10.174508000
H	4.888481000	-1.093358000	11.744331000

[NHC(F)→AuOAc]

E= -1707.262434

Cl	6.343425000	6.053377000	3.890903000
Cl	5.618327000	7.698622000	6.992690000
N	5.975561000	4.079250000	5.729737000
N	5.558669000	5.029411000	7.520319000
C	5.694129000	3.773078000	7.022036000

C	5.736481000	6.061776000	6.614634000
C	6.015202000	5.428441000	5.420621000
Au	5.524541000	2.047225000	7.918320000
O	5.346848000	0.211487000	8.757021000
C	5.209152000	0.226276000	10.075637000
O	5.183272000	1.239125000	10.771985000
C	5.085698000	-1.171710000	10.657578000
H	5.979932000	-1.760468000	10.408410000
H	4.224702000	-1.689500000	10.211821000
H	4.966770000	-1.117618000	11.744655000
F	6.202937000	3.123273000	4.794479000
F	5.258613000	5.262125000	8.820609000

[NHC(Br)→AuOAc]

E= -6655.309144

Cl	6.270480000	6.121072000	3.902277000
Cl	5.656596000	7.661474000	7.001701000
N	5.966905000	4.045810000	5.655748000
N	5.593588000	4.985597000	7.540283000
C	5.720690000	3.744684000	6.970334000
C	5.753417000	6.020079000	6.621538000
C	5.992966000	5.418988000	5.412086000
Au	5.573916000	2.016417000	7.875581000
O	5.427789000	0.210769000	8.785673000
C	5.176793000	0.255266000	10.085633000
O	5.033207000	1.282185000	10.747612000
C	5.079530000	-1.132003000	10.699253000
H	6.015598000	-1.683352000	10.531551000

H	4.277839000	-1.702834000	10.209396000
H	4.879030000	-1.056126000	11.773101000
Br	5.245927000	5.214825000	9.345358000
Br	6.232975000	2.750258000	4.360875000

[NHC(C(CH3)3)→AuOAc]

E= -1823.186027

Cl	5.840455000	6.651384000	3.530442000
Cl	5.712499000	8.237565000	6.312667000
O	5.870262000	0.829078000	8.703787000
O	5.679939000	1.984759000	10.647808000
N	5.924527000	4.496976000	5.331016000
N	5.837699000	5.595254000	7.259478000
C	5.898763000	4.339366000	6.699234000
C	5.812049000	6.534728000	6.232512000
C	5.865759000	5.857473000	5.042364000
C	5.763905000	0.928877000	10.015194000
C	5.755000000	-0.427324000	10.703545000
H	6.685843000	-0.967190000	10.478292000
H	4.927183000	-1.039015000	10.317688000
H	5.651968000	-0.301873000	11.786579000
Au	5.893415000	2.615900000	7.709225000
C	5.816429000	5.817217000	8.780361000
C	7.096484000	5.212313000	9.375413000
C	4.550476000	5.163102000	9.351997000
H	3.650156000	5.570833000	8.869766000
H	4.563073000	4.070178000	9.246346000
H	4.498097000	5.382000000	10.427354000

H	7.148167000	4.125406000	9.229327000
H	7.099776000	5.395907000	10.458412000
H	7.989231000	5.683014000	8.938359000
C	5.789262000	7.303325000	9.157388000
H	4.878746000	7.814297000	8.823310000
H	5.802992000	7.337792000	10.255072000
H	6.668075000	7.852790000	8.799326000
C	6.008386000	3.305747000	4.371966000
C	4.749844000	2.446387000	4.559217000
C	7.293006000	2.523137000	4.684123000
H	8.178989000	3.159796000	4.546975000
H	7.293355000	2.130691000	5.710191000
H	7.367393000	1.673828000	3.990873000
H	4.673171000	2.057265000	5.583979000
H	4.795657000	1.592662000	3.868786000
H	3.844790000	3.027443000	4.330578000
C	6.073988000	3.728433000	2.899413000
H	6.953886000	4.341113000	2.670248000
H	6.156655000	2.800327000	2.317342000
H	5.170386000	4.249459000	2.563242000

[NHC(CF3)→AuOAc]

E= -2182.761922

Cl	6.010908000	6.469724000	3.513150000
Cl	5.800189000	8.182537000	6.368473000
O	5.878039000	0.855146000	8.826888000
O	5.811417000	2.044238000	10.758453000
N	5.954114000	4.432811000	5.413071000

N	5.816734000	5.548291000	7.271136000
C	5.880990000	4.265701000	6.777879000
C	5.851926000	6.496343000	6.233469000
C	5.938362000	5.795810000	5.064271000
C	5.842256000	0.977708000	10.148568000
C	5.843072000	-0.369510000	10.849809000
H	6.738044000	-0.940403000	10.564459000
H	4.971189000	-0.958129000	10.530692000
H	5.820383000	-0.229394000	11.935506000
Au	5.877179000	2.602920000	7.812070000
C	5.727826000	5.788257000	8.724535000
F	5.666205000	7.105357000	8.963208000
F	4.627423000	5.213583000	9.213239000
F	6.806053000	5.292811000	9.333939000
C	6.040302000	3.268401000	4.523597000
F	6.091867000	3.667117000	3.246892000
F	7.144310000	2.562307000	4.794251000
F	4.966209000	2.486682000	4.682364000

[NHC(CH3)→AuOAc]

E= -1587.587929

Cl	5.966838000	6.404922000	3.544925000
Cl	5.802725000	8.062241000	6.657129000
O	5.893372000	0.748595000	8.818921000
O	5.787654000	2.085896000	10.648768000
N	5.941779000	4.396185000	5.383810000
N	5.840719000	5.417122000	7.300070000
C	5.893351000	4.173389000	6.732099000

C	5.856146000	6.399467000	6.321450000
C	5.919816000	5.756993000	5.113670000
C	6.007174000	3.346365000	4.378149000
H	6.925330000	3.443822000	3.783893000
H	5.135693000	3.400815000	3.712414000
H	6.008739000	2.390408000	4.914279000
C	5.777356000	5.666358000	8.736694000
H	6.647217000	6.255777000	9.054778000
H	5.780499000	4.693351000	9.245831000
H	4.857561000	6.212613000	8.983340000
C	5.836082000	0.971563000	10.118634000
C	5.835162000	-0.310403000	10.934695000
H	6.743962000	-0.890844000	10.720885000
H	4.978622000	-0.936717000	10.647356000
H	5.784777000	-0.079414000	12.003976000
Au	5.894395000	2.478873000	7.732893000

[NHC(H)→AuOAc]

E= -1509.05122

Cl	6.269493000	6.117301000	3.916278000
Cl	5.642133000	7.658670000	7.072607000
N	5.964860000	4.061412000	5.668349000
N	5.588941000	4.986190000	7.559682000
C	5.718934000	3.760816000	6.975444000
C	5.747425000	6.021491000	6.650488000
C	5.988093000	5.430298000	5.439619000
Au	5.575383000	2.022811000	7.861225000
O	5.433592000	0.197470000	8.745449000

C	5.185398000	0.250176000	10.043833000
O	5.045727000	1.284385000	10.698278000
C	5.084746000	-1.129847000	10.672735000
H	6.018547000	-1.686233000	10.508824000
H	4.279897000	-1.703121000	10.190881000
H	4.886980000	-1.042243000	11.746234000
H	5.397679000	5.105693000	8.550035000
H	6.111865000	3.353794000	4.956321000

[NHC(Ph)→AuOAc]

E= -1970.704822

Cl	-4.426402000	0.701618000	-0.464940000
Cl	-2.510345000	3.600081000	-0.515070000
O	2.764419000	-1.911756000	0.419706000
O	3.768356000	-0.456933000	-1.007402000
N	-1.882474000	-0.196128000	-0.004421000
N	-0.677296000	1.620525000	-0.015772000
C	-0.592277000	0.255435000	0.111992000
C	-2.002854000	2.009517000	-0.213728000
C	-2.758998000	0.870297000	-0.203033000
C	3.785236000	-1.452417000	-0.278775000
C	5.039538000	-2.293417000	-0.094243000
H	4.824502000	-3.349785000	-0.307287000
H	5.370058000	-2.237322000	0.953190000
H	5.838345000	-1.932214000	-0.750721000
C	0.448587000	2.509154000	0.094924000
C	0.408164000	3.552435000	1.024289000
C	1.578443000	2.290511000	-0.696355000

C	1.513066000	4.393999000	1.150962000
C	2.685023000	3.126679000	-0.544183000
C	2.652061000	4.181055000	0.370174000
H	-0.470648000	3.692802000	1.654076000
H	1.613603000	1.458116000	-1.398670000
H	1.487908000	5.207475000	1.877574000
H	3.577590000	2.932386000	-1.139446000
H	3.519665000	4.833033000	0.483551000
C	-2.266332000	-1.577521000	0.080117000
C	-1.777440000	-2.483026000	-0.863311000
C	-3.114304000	-1.993342000	1.108515000
C	-2.142223000	-3.826369000	-0.768220000
C	-3.478531000	-3.337663000	1.189089000
C	-2.992776000	-4.254040000	0.253703000
H	-1.112946000	-2.134473000	-1.653849000
H	-3.472385000	-1.273105000	1.844958000
H	-1.756857000	-4.540093000	-1.497473000
H	-4.135294000	-3.670116000	1.994158000
H	-3.274365000	-5.305774000	0.324087000
Au	1.058619000	-0.801095000	0.286172000

[NHC(Si(CH3)3)→AuOAc]

E= -2325.899344

Cl	5.692590000	7.082785000	3.821147000
Cl	5.020837000	8.305014000	6.891608000
O	6.626400000	0.916992000	8.393418000
O	6.173902000	1.739732000	10.459019000
N	6.036296000	4.854238000	5.407663000

N	5.594280000	5.653039000	7.440876000
C	5.953263000	4.522617000	6.741238000
C	5.453374000	6.697023000	6.531642000
C	5.724160000	6.207553000	5.286202000
C	6.490630000	0.818455000	9.698962000
C	6.768512000	-0.585253000	10.214324000
H	7.790099000	-0.888099000	9.943901000
H	6.084051000	-1.301344000	9.737619000
H	6.645778000	-0.621961000	11.301951000
Si	5.382964000	5.584234000	9.300169000
C	7.037081000	5.116409000	10.035232000
H	7.055322000	5.441029000	11.088068000
H	7.185135000	4.027148000	10.017231000
H	7.870557000	5.610369000	9.515404000
C	4.893825000	7.287620000	9.921509000
H	3.932055000	7.641706000	9.528543000
H	4.785900000	7.178027000	11.013554000
H	5.653708000	8.058743000	9.740554000
C	3.999237000	4.380379000	9.662573000
H	3.175112000	4.474521000	8.940870000
H	4.366638000	3.344202000	9.669496000
H	3.598049000	4.601669000	10.664702000
Si	6.475096000	3.759796000	3.979896000
C	6.832004000	2.005393000	4.505588000
H	7.689723000	1.919106000	5.185283000
H	5.973636000	1.507283000	4.974859000
H	7.077251000	1.456851000	3.578831000
C	4.985357000	3.768176000	2.840842000

H	5.184766000	3.101253000	1.987699000
H	4.100263000	3.378575000	3.365335000
H	4.743108000	4.762404000	2.445353000
C	8.019214000	4.498399000	3.213861000
H	8.839197000	4.516310000	3.947047000
H	8.340078000	3.863070000	2.373748000
H	7.873511000	5.516929000	2.833055000
Au	6.276049000	2.767493000	7.582740000

[NHC(SiH3)→AuOAc]

E= -2090.171184

Cl	5.643080000	7.097798000	3.812273000
Cl	4.938755000	8.228047000	7.044206000
O	6.675131000	0.952059000	8.403104000
O	6.177816000	1.938400000	10.385207000
N	6.026517000	4.889120000	5.358209000
N	5.585371000	5.587485000	7.401759000
C	5.964997000	4.490984000	6.670701000
C	5.408766000	6.673738000	6.546180000
C	5.682557000	6.239362000	5.280162000
C	6.513742000	0.959611000	9.714814000
C	6.788799000	-0.396629000	10.343004000
H	7.812634000	-0.719218000	10.106264000
H	6.108650000	-1.149480000	9.919631000
H	6.655945000	-0.345136000	11.428751000
Au	6.316314000	2.748613000	7.510148000
Si	5.401732000	5.415344000	9.210039000
H	4.329363000	4.422953000	9.457227000

H	6.728519000	5.052566000	9.761194000
H	4.988077000	6.778711000	9.648164000
Si	6.479402000	3.828526000	3.968885000
H	6.752436000	2.499321000	4.565264000
H	5.325261000	3.816939000	3.028737000
H	7.677744000	4.433166000	3.325122000

[NHC(CF3)→AuCl]

E= -2414.49584

C	-0.031208000	14.564459000	6.372533000
C	0.607308000	14.860182000	8.573774000
N	0.849304000	15.196051000	7.230263000
Cl	-0.246142000	14.821127000	2.148607000
Au	-0.131702000	14.684947000	4.401713000
C	-0.445260000	13.999719000	8.574858000
N	-0.824204000	13.827977000	7.231990000
Cl	1.473356000	15.430912000	9.908927000
Cl	-1.175132000	13.265776000	9.911652000
C	-1.940948000	12.952736000	6.866557000
F	-2.143737000	12.921274000	5.560048000
F	-1.682028000	11.704407000	7.301261000
F	-3.060285000	13.390602000	7.474578000
C	1.928634000	16.116128000	6.862553000
F	1.722760000	17.300813000	7.469570000
F	3.101103000	15.614666000	7.296354000
F	1.998181000	16.307223000	5.555753000

[NHC(Br)→AuCl]

E= -6887.040696

C	0.000000000	0.000000000	-0.218962000
C	0.000281000	0.685648000	-2.419986000
N	0.000064000	1.068514000	-1.079596000
Cl	0.000000000	0.000000000	4.017863000
Au	0.000000000	0.000000000	1.752677000
C	-0.000281000	-0.685648000	-2.419986000
N	-0.000064000	-1.068514000	-1.079596000
Cl	0.000624000	1.756472000	-3.724611000
Cl	-0.000624000	-1.756472000	-3.724611000
Br	0.000000000	2.825115000	-0.495149000
Br	0.000000000	-2.825115000	-0.495149000

[NHC(C(CH3)3)→AuCl]

E= -2054.915514

C	0.016027000	14.551802000	6.455567000
C	0.538824000	14.849814000	8.631314000
N	0.899971000	15.167246000	7.324836000
Cl	0.190858000	14.852298000	2.173367000
Au	0.088460000	14.685598000	4.449352000
C	-0.562485000	14.042359000	8.570408000
N	-0.886413000	13.857406000	7.228514000
Cl	1.248808000	15.313370000	10.113980000
Cl	-1.348575000	13.409735000	9.949501000
C	-2.068562000	13.005820000	6.776190000
C	2.062335000	16.041078000	6.836255000
C	-1.836118000	11.565013000	7.266067000
H	-2.673707000	10.940330000	6.927163000

H	-0.913701000	11.160853000	6.825919000
H	-1.773769000	11.480193000	8.355621000
C	-3.354687000	13.629644000	7.347717000
H	-4.213300000	13.033598000	7.009847000
H	-3.375900000	13.658283000	8.441768000
H	-3.481218000	14.651766000	6.964067000
C	-2.228186000	12.948451000	5.256920000
H	-1.364859000	12.496355000	4.752519000
H	-3.103655000	12.312124000	5.059085000
H	-2.420887000	13.931618000	4.809265000
C	2.901756000	16.612069000	7.986160000
H	2.331428000	17.278071000	8.644149000
H	3.390604000	15.836230000	8.586907000
H	3.693143000	17.212067000	7.516499000
C	2.993400000	15.175084000	5.975376000
H	3.834466000	15.793700000	5.632798000
H	3.397712000	14.338438000	6.563503000
H	2.483261000	14.773283000	5.089396000
C	1.482567000	17.230731000	6.057457000
H	2.311016000	17.866567000	5.715663000
H	0.913184000	16.909676000	5.174633000
H	0.828200000	17.834335000	6.703059000

[NHC(CH3)→AuCl]

E= -1819.317994

C	0.018913000	14.503254000	6.463551000

C	0.477601000	15.026586000	8.621570000
N	0.838449000	15.217409000	7.295791000
Cl	0.168972000	14.311697000	2.211528000
Au	0.088954000	14.414124000	4.481063000
C	-0.592648000	14.173196000	8.621884000
N	-0.859647000	13.863684000	7.296278000
C	1.937631000	16.061108000	6.848633000
H	2.887292000	15.700948000	7.265664000
H	1.965200000	16.003267000	5.754410000
H	1.772069000	17.099783000	7.163636000
C	-1.927257000	12.980019000	6.849805000
H	-1.877497000	12.939972000	5.755568000
H	-1.787562000	11.974093000	7.267038000
H	-2.902789000	13.372937000	7.165139000
Cl	1.275559000	15.758326000	9.928961000
Cl	-1.483240000	13.558598000	9.929769000

[NHC(Cl)→AuCl]

E= -2659.539142

C	0.000000000	14.527000000	6.454606000
C	0.539406000	14.949787000	8.663185000
N	0.838689000	15.183385000	7.319902000
Cl	0.000000000	14.527000000	2.222755000
Au	0.000000000	14.527000000	4.485928000
C	-0.539406000	14.104213000	8.663185000
N	-0.838689000	13.870615000	7.319902000
Cl	1.388503000	15.615064000	9.959261000
Cl	-1.388503000	13.438936000	9.959261000

Cl	2.103253000	16.173074000	6.801506000
Cl	-2.103253000	12.880926000	6.801506000

[NHC(F)→AuCl]

E= -1938.994745

C	0.000000000	14.527000000	6.449731000
C	0.542988000	14.952682000	8.671673000
N	0.814503000	15.164096000	7.330067000
Cl	0.000000000	14.527000000	2.221983000
Au	0.000000000	14.527000000	4.482206000
C	-0.542988000	14.101318000	8.671673000
N	-0.814503000	13.889904000	7.330067000
Cl	1.410636000	15.632517000	9.944874000
Cl	-1.410636000	13.421483000	9.944874000
F	-1.832891000	13.093464000	6.923921000
F	1.832891000	15.960536000	6.923921000

[NHC(H)→AuCl]

E= -1740.782327

C	0.000000000	14.527000000	6.480772000
C	0.538861000	14.948792000	8.662016000
N	0.841508000	15.185356000	7.328547000
Cl	0.000000000	14.527000000	2.240181000
Au	0.000000000	14.527000000	4.508577000
C	-0.538861000	14.105208000	8.662016000
N	-0.841508000	13.868644000	7.328547000
Cl	1.405368000	15.626969000	9.950349000
Cl	-1.405368000	13.427031000	9.950349000

H	-1.598915000	13.276085000	7.004437000
H	1.598915000	15.777915000	7.004437000

[NHC(Ph)→AuCl]

E= -2202.434874

C	0.000000000	14.527000000	6.443152000
C	0.525415000	14.964028000	8.615474000
N	0.837983000	15.222165000	7.280270000
Cl	0.000000000	14.527000000	2.186365000
Au	0.000000000	14.527000000	4.461636000
C	-0.525415000	14.089972000	8.615474000
N	-0.837983000	13.831835000	7.280270000
Cl	1.310447000	15.673711000	9.941259000
Cl	-1.310447000	13.380289000	9.941259000
C	1.882843000	16.099482000	6.830599000
C	3.207553000	15.822636000	7.174305000
C	1.556819000	17.208789000	6.047866000
C	4.218295000	16.675519000	6.730284000
C	2.577060000	18.048914000	5.601233000
C	3.905084000	17.786521000	5.943969000
H	3.444415000	14.940917000	7.770624000
H	0.516336000	17.399187000	5.785033000
H	5.255912000	16.461354000	6.990077000
H	2.329193000	18.910613000	4.980245000
H	4.699586000	18.446184000	5.591877000
C	-1.882843000	12.954518000	6.830599000
C	-1.556819000	11.845211000	6.047866000
C	-3.207553000	13.231364000	7.174305000

C	-2.577060000	11.005086000	5.601233000
C	-4.218295000	12.378481000	6.730284000
C	-3.905084000	11.267479000	5.943969000
H	-0.516336000	11.654813000	5.785033000
H	-3.444415000	14.113083000	7.770624000
H	-2.329193000	10.143387000	4.980245000
H	-5.255912000	12.592646000	6.990077000
H	-4.699586000	10.607816000	5.591877000

[NHC(Si(CH3)3)→AuCl]

E= -2557.627943

C	0.271435000	0.057717000	0.000626000
C	2.510194000	-0.031497000	-0.000583000
N	1.347348000	-0.800763000	0.000434000
C	2.151688000	1.285224000	-0.000743000
N	0.760797000	1.348121000	0.000128000
Cl	4.102007000	-0.646886000	-0.001705000
Cl	3.226337000	2.607580000	-0.002610000
Si	1.335287000	-2.655896000	0.001427000
C	-0.389124000	-3.364411000	0.004247000
H	-0.260840000	-4.461464000	0.004776000
H	-0.973642000	-3.092935000	0.892791000
H	-0.976217000	-3.094059000	-0.882937000
C	2.215019000	-3.177166000	-1.570606000
H	1.674560000	-2.804152000	-2.453209000
H	3.253930000	-2.829274000	-1.627579000
H	2.221197000	-4.276784000	-1.627455000
C	2.219090000	-3.175424000	1.571784000

H	3.259098000	-2.830145000	1.624341000
H	1.682689000	-2.798802000	2.455333000
H	2.222506000	-4.274906000	1.631369000
Si	-0.401962000	2.801862000	0.001411000
H	-0.734554000	2.717022000	-2.458911000
C	-1.397071000	2.725543000	-1.580660000
H	-2.050793000	1.844479000	-1.625465000
H	-2.059851000	1.843411000	1.619377000
C	-1.401175000	2.721053000	1.580755000
H	-0.740633000	2.703801000	2.460378000
H	-2.028655000	3.625837000	-1.644448000
H	-2.027704000	3.624602000	1.648374000
H	-0.175993000	5.210026000	0.008891000
H	1.202809000	4.533049000	0.897970000
C	0.576348000	4.403688000	0.006100000
H	1.202619000	4.538870000	-0.885004000
Au	-1.663759000	-0.410809000	-0.000411000
Cl	-3.893963000	-0.917637000	-0.002465000

[NHC(SiH3)→AuCl]

E= -2321.901363

Cl	5.643080000	7.097798000	3.812273000
Cl	4.938755000	8.228047000	7.044206000
O	6.675131000	0.952059000	8.403104000
O	6.177816000	1.938400000	10.385207000
N	6.026517000	4.889120000	5.358209000
N	5.585371000	5.587485000	7.401759000
C	5.964997000	4.490984000	6.670701000

C	5.408766000	6.673738000	6.546180000
C	5.682557000	6.239362000	5.280162000
C	6.513742000	0.959611000	9.714814000
C	6.788799000	-0.396629000	10.343004000
H	7.812634000	-0.719218000	10.106264000
H	6.108650000	-1.149480000	9.919631000
H	6.655945000	-0.345136000	11.428751000
Au	6.316314000	2.748613000	7.510148000
Si	5.401732000	5.415344000	9.210039000
H	4.329363000	4.422953000	9.457227000
H	6.728519000	5.052566000	9.761194000
H	4.988077000	6.778711000	9.648164000
Si	6.479402000	3.828526000	3.968885000
H	6.752436000	2.499321000	4.565264000
H	5.325261000	3.816939000	3.028737000
H	7.677744000	4.433166000	3.325122000

[NHC(CH3)→AgOAc]

E= -1598.798567

Ag	5.899674000	2.336420000	7.644725000
Cl	5.961669000	6.552508000	3.623501000
Cl	5.798937000	8.013452000	6.829208000
O	5.898649000	0.573949000	8.785592000
O	5.794509000	2.179064000	10.370894000
N	5.942498000	4.432357000	5.339119000
N	5.842519000	5.329811000	7.308516000
C	5.896421000	4.124456000	6.668070000
C	5.854655000	6.372617000	6.395328000

C	5.917945000	5.805811000	5.149000000
C	6.008466000	3.446319000	4.271306000
H	6.925401000	3.580644000	3.682253000
H	5.136476000	3.538839000	3.610353000
H	6.012479000	2.458507000	4.746084000
C	5.780453000	5.490795000	8.758929000
H	6.649105000	6.063442000	9.109503000
H	5.785655000	4.490739000	9.215483000
H	4.860573000	6.021380000	9.037635000
C	5.839160000	0.981710000	10.020778000
C	5.827067000	-0.133864000	11.054100000
H	6.732745000	-0.747964000	10.948022000
H	4.968110000	-0.796355000	10.875537000
H	5.774285000	0.277694000	12.067816000

[NHC(Cl)→AgOAc]

E= -2439.018699

Ag	5.753425000	2.006342000	7.576876000
Cl	6.167562000	6.471225000	3.854588000
Cl	5.612618000	7.773929000	7.087223000
N	5.995905000	4.278768000	5.480323000
N	5.662832000	5.062237000	7.420553000
C	5.809549000	3.870796000	6.769853000
C	5.752366000	6.171185000	6.580543000
C	5.968223000	5.664568000	5.323295000
Cl	6.237229000	3.202467000	4.197362000
Cl	5.397987000	5.168474000	9.088615000
O	5.722357000	0.013330000	8.254146000

C	5.518007000	0.124836000	9.536054000
O	5.384441000	1.211974000	10.130782000
C	5.449473000	-1.195091000	10.287373000
H	6.384235000	-1.754984000	10.141760000
H	4.637812000	-1.813455000	9.878187000
H	5.281999000	-1.022800000	11.355972000

[NHC(F)→AgOAc]

E= -1718.476991

Ag	5.884873000	2.546805000	7.933291000
Cl	5.974077000	6.267785000	3.477699000
Cl	5.805090000	8.173599000	6.510439000
O	5.897738000	0.595130000	8.784364000
O	5.797015000	2.060263000	10.482806000
N	5.935651000	4.459316000	5.519644000
N	5.838772000	5.552153000	7.257850000
C	5.886400000	4.267571000	6.851795000
C	5.855805000	6.507991000	6.258132000
C	5.920961000	5.772755000	5.089183000
C	5.841552000	0.888292000	10.047974000
C	5.832514000	-0.297182000	10.996464000
H	6.738117000	-0.900962000	10.842683000
H	4.972850000	-0.944353000	10.771901000
H	5.782607000	0.039538000	12.037348000
F	5.777210000	5.895805000	8.574597000
F	5.996597000	3.418349000	4.638792000

[NHC(C(CH3)3)→AgOAc]

E= -1834.401333

Cl	5.772446000	6.551014000	3.712577000
Cl	5.384829000	7.837246000	6.712453000
N	5.939619000	4.265214000	5.311767000
N	5.688585000	5.127202000	7.320253000
C	5.821465000	3.939741000	6.642178000
C	5.652822000	6.177101000	6.409014000
C	5.810795000	5.642061000	5.160177000
C	6.238063000	3.307365000	4.172330000
C	5.028243000	3.274200000	3.226421000
H	4.819882000	4.250916000	2.774435000
H	5.225516000	2.559766000	2.415189000
H	4.133193000	2.936697000	3.767474000
C	7.521735000	3.782963000	3.465812000
H	8.361275000	3.805211000	4.175100000
H	7.769695000	3.067526000	2.670081000
H	7.422992000	4.771631000	3.007020000
C	6.505849000	1.887949000	4.677040000
H	6.812150000	1.289194000	3.807090000
H	7.314759000	1.854004000	5.417957000
H	5.613386000	1.411786000	5.108594000
C	5.656173000	5.307294000	8.832400000
C	5.909786000	3.991040000	9.571038000
H	6.005010000	4.242292000	10.637716000
H	6.846418000	3.512368000	9.255161000
C	4.269033000	5.832004000	9.232584000
H	4.031976000	6.799564000	8.774208000
H	3.496446000	5.101553000	8.955653000

H	4.236795000	5.956123000	10.323854000
C	6.792221000	6.272449000	9.220932000
H	6.795682000	6.380970000	10.313809000
H	7.764678000	5.856422000	8.920463000
H	6.688315000	7.271981000	8.787336000
Ag	5.149360000	2.117071000	7.379481000
H	5.075616000	3.276337000	9.487936000
O	4.336433000	0.281814000	8.011750000
C	3.529939000	0.533172000	9.001894000
O	3.302499000	1.667038000	9.466135000
C	2.849463000	-0.698205000	9.584434000
H	3.607869000	-1.413833000	9.932696000
H	2.266182000	-1.204711000	8.802110000
H	2.191616000	-0.420289000	10.415040000

[NHC(Br)→AgOAc]

E= -6666.520276

Ag	-1.641105000	-0.582425000	0.020420000
Cl	4.184424000	-0.886209000	0.018322000
Cl	3.251788000	2.503251000	-0.056337000
O	-3.663699000	-1.178550000	0.037414000
O	-3.790243000	1.069573000	-0.041770000
N	1.447111000	-0.915940000	0.024182000
N	0.885280000	1.133870000	-0.020994000
C	0.340930000	-0.117364000	0.008263000
C	2.276966000	1.124857000	-0.023358000
C	2.641420000	-0.198767000	0.005815000
C	-4.323060000	-0.056992000	-0.002950000

C	-5.836450000	-0.207645000	0.003874000
H	-6.152610000	-0.710715000	0.929005000
H	-6.151733000	-0.846338000	-0.833203000
H	-6.323052000	0.770925000	-0.068929000
Br	-0.153267000	2.675796000	-0.053932000
Br	1.354691000	-2.770015000	0.066464000

[NHC(CF3)→AgOAc]

E= -2193.979677

Ag	5.706517000	2.681361000	8.203240000
Cl	6.377036000	6.165222000	3.557549000
Cl	5.843416000	8.198438000	6.276224000
O	4.802661000	0.951038000	9.320192000
O	7.000407000	1.259232000	9.519614000
N	5.992556000	4.380590000	5.629666000
N	5.659173000	5.652702000	7.330924000
C	5.745519000	4.321520000	6.984337000
C	5.858796000	6.507011000	6.232135000
C	6.069799000	5.702077000	5.155710000
C	5.940945000	0.614369000	9.794536000
C	6.008237000	-0.590462000	10.708666000
H	5.626219000	-1.474352000	10.178744000
H	5.354366000	-0.428436000	11.577135000
H	7.034091000	-0.774210000	11.045615000
C	5.388461000	6.164302000	8.669876000
F	4.290632000	6.944335000	8.639582000
F	5.189967000	5.177011000	9.535246000
F	6.426743000	6.912466000	9.087722000

C	6.158206000	3.230944000	4.747199000
F	7.387238000	3.254269000	4.198158000
F	5.998990000	2.088215000	5.404274000
F	5.250428000	3.292420000	3.753863000

[NHC(H)→AgOAc]

E= -1520.260838

Ag	5.896026000	2.417494000	7.742036000
Cl	5.965102000	6.463681000	3.557662000
Cl	5.799206000	8.067715000	6.739797000
O	5.897612000	0.608779000	8.801735000
O	5.795019000	2.145485000	10.449282000
N	5.941077000	4.443285000	5.380965000
N	5.842074000	5.401839000	7.280597000
C	5.894831000	4.165228000	6.712593000
C	5.854971000	6.421597000	6.341383000
C	5.918667000	5.806035000	5.119539000
C	5.839323000	0.964196000	10.054562000
C	5.828252000	-0.194088000	11.039844000
H	6.733633000	-0.803480000	10.907324000
H	4.968726000	-0.848253000	10.835183000
H	5.776900000	0.175424000	12.069672000
H	5.798442000	5.543397000	8.285983000
H	5.986918000	3.725956000	4.664919000

[NHC(Ph)→AgOAc]

E= -1981.916359

Ag	5.711303000	2.444124000	7.748121000
Cl	6.180304000	6.526737000	3.632575000
Cl	5.949894000	8.130547000	6.699185000
O	5.809946000	0.630196000	8.784876000
O	7.357803000	1.799747000	9.944675000
N	5.834121000	4.470697000	5.415326000
N	5.676471000	5.471505000	7.336451000
C	5.684684000	4.230794000	6.755144000
C	5.819498000	6.469767000	6.372936000
C	5.916151000	5.839436000	5.162009000
C	6.690123000	0.768779000	9.734721000
C	6.856826000	-0.461175000	10.616626000
H	7.068322000	-1.343852000	9.996990000
H	5.915806000	-0.661462000	11.149488000
H	7.663676000	-0.309900000	11.342003000
C	5.510786000	5.685709000	8.749680000
C	4.501130000	6.539815000	9.202603000
C	6.334979000	5.001290000	9.645993000
C	4.326320000	6.718463000	10.574713000
C	6.135091000	5.173986000	11.016614000
C	5.140611000	6.035662000	11.482318000
H	3.848406000	7.045046000	8.490435000
H	7.102606000	4.311574000	9.292495000
H	3.537619000	7.381317000	10.933726000
H	6.762774000	4.616404000	11.712490000
H	4.991668000	6.169506000	12.554997000
C	5.890295000	3.436368000	4.421539000
C	6.877208000	2.452977000	4.517125000

C	4.949393000	3.415343000	3.389570000
C	6.915147000	1.431656000	3.566871000
C	5.003061000	2.394710000	2.440077000
C	5.982621000	1.402660000	2.527911000
H	7.601996000	2.491195000	5.330917000
H	4.174634000	4.181082000	3.340873000
H	7.679710000	0.657413000	3.642006000
H	4.266691000	2.369513000	1.635561000
H	6.016324000	0.602827000	1.786681000

[NHC(Si(CH3)3)→AgOAc]

E= -2337.109675

Ag	6.286687000	2.715087000	7.596339000
Cl	5.684156000	7.112808000	3.819411000
Cl	5.012083000	8.329248000	6.899655000
O	6.661691000	0.793042000	8.341603000
O	6.182776000	1.767897000	10.321249000
N	6.028999000	4.884204000	5.407665000
N	5.589677000	5.673071000	7.434391000
C	5.948840000	4.542400000	6.737558000
C	5.446209000	6.722182000	6.532297000
C	5.716776000	6.236108000	5.284587000
C	6.506360000	0.780954000	9.634033000
C	6.755944000	-0.574302000	10.281260000
H	7.779798000	-0.908871000	10.060924000
H	6.074909000	-1.322859000	9.851602000
H	6.609325000	-0.518518000	11.365332000
Si	5.382215000	5.592120000	9.288190000

C	7.039735000	5.105295000	10.002707000
H	7.048767000	5.366300000	11.073124000
H	7.203234000	4.019881000	9.929490000
H	7.868313000	5.640401000	9.516915000
C	4.892668000	7.284410000	9.935531000
H	3.929553000	7.641011000	9.548076000
H	4.788058000	7.163996000	11.026599000
H	5.650920000	8.058242000	9.759160000
C	4.009193000	4.370693000	9.631460000
H	3.163580000	4.500191000	8.940780000
H	4.374828000	3.334280000	9.582791000
H	3.639536000	4.539698000	10.655567000
Si	6.469149000	3.781596000	3.992550000
C	6.820922000	2.038600000	4.561559000
H	7.677486000	1.963264000	5.245113000
H	5.959535000	1.548015000	5.034809000
H	7.070898000	1.465332000	3.651448000
C	4.984938000	3.774048000	2.846942000
H	5.187763000	3.100934000	1.999573000
H	4.097182000	3.389538000	3.370609000
H	4.744913000	4.765558000	2.442723000
C	8.014971000	4.507084000	3.218315000
H	8.834643000	4.536332000	3.951433000
H	8.337171000	3.862435000	2.385929000
H	7.867284000	5.520752000	2.824900000

[NHC(SiH3)→AgOAc]

E= -2101.380366

Ag	5.881866000	2.457834000	7.752158000
Cl	5.945273000	6.459214000	3.542021000
Cl	5.851310000	8.116422000	6.646974000
O	5.875894000	0.632792000	8.772422000
O	5.817644000	2.049843000	10.531108000
N	5.920435000	4.438148000	5.373865000
N	5.861941000	5.470031000	7.308876000
C	5.888887000	4.224864000	6.731776000
C	5.876524000	6.448513000	6.317949000
C	5.912907000	5.807190000	5.113154000
C	5.841812000	0.902523000	10.047595000
C	5.833406000	-0.325443000	10.946037000
H	6.730357000	-0.931846000	10.755084000
H	4.964159000	-0.954937000	10.707726000
H	5.801489000	-0.032269000	12.000930000
Si	5.814321000	5.750943000	9.106046000
H	5.813638000	4.394367000	9.713305000
H	7.020078000	6.565382000	9.426637000
H	4.577008000	6.539234000	9.366083000
Si	5.963602000	3.121565000	4.140254000
H	5.957831000	1.862914000	4.926126000
H	4.756933000	3.276783000	3.281939000
H	7.206492000	3.302086000	3.340586000

[NHC(Br)→AgCl]

E= -6898.2495995

Ag	5.915313000	2.258525000	7.645708000
Cl	5.901299000	6.473236000	3.632654000

Cl	5.832293000	8.014238000	6.792544000
N	5.910830000	4.400217000	5.417519000
N	5.869146000	5.331827000	7.327807000
C	5.897484000	4.094735000	6.748940000
C	5.864982000	6.372436000	6.401351000
C	5.891949000	5.770763000	5.167605000
Cl	5.934523000	0.208781000	8.647698000
Br	5.951066000	3.101190000	4.094420000
Br	5.840211000	5.574576000	9.166203000

[NHC(CF3)→AgCl]

E= -2425.7074201

Ag	5.893781000	2.194812000	7.623755000
Cl	5.927194000	6.519227000	3.671188000
Cl	5.856386000	7.991418000	6.774892000
N	5.914992000	4.370087000	5.403674000
N	5.870488000	5.289830000	7.343199000
C	5.893122000	4.055789000	6.740530000
C	5.878415000	6.340668000	6.410504000
C	5.906361000	5.757122000	5.180182000
Cl	5.894396000	0.136481000	8.601420000
C	5.943990000	3.408548000	4.299014000
F	7.047800000	3.616685000	3.558733000
F	5.947210000	2.159941000	4.742888000
F	4.864507000	3.596842000	3.518543000
C	5.842103000	5.536966000	8.786736000
F	4.737963000	6.241358000	9.094467000
F	5.839818000	4.403391000	9.472986000

F	6.921304000	6.261079000	9.134186000

[NHC(Cl)→AgCl]

E= -2425.7074201

Ag	5.901038000	2.263180000	7.653136000
Cl	5.963574000	6.459451000	3.623840000
Cl	5.800283000	8.015514000	6.788290000
N	5.940056000	4.401306000	5.421953000
N	5.842023000	5.335228000	7.321211000
C	5.894005000	4.094317000	6.752308000
C	5.854658000	6.376902000	6.393316000
C	5.918135000	5.771982000	5.163108000
Cl	5.908916000	0.217698000	8.659776000
Cl	6.016279000	3.223789000	4.210925000
Cl	5.769428000	5.575451000	8.993330000

[NHC(F)→AgCl]

E= -1950.2062622

Ag	5.901046000	2.261659000	7.651302000
Cl	5.964781000	6.437477000	3.608453000
Cl	5.798962000	8.013805000	6.824234000
N	5.938515000	4.424472000	5.445966000
N	5.843369000	5.328681000	7.290561000
C	5.894060000	4.092211000	6.752889000
C	5.854377000	6.385449000	6.397181000
C	5.918294000	5.777774000	5.157505000
Cl	5.909333000	0.216527000	8.655088000
F	5.999810000	3.485447000	4.464226000

F	5.784709000	5.529538000	8.634246000

[NHC(Me)→AgCl]

E= -1830 .5259706

Ag	1.981453000	-0.113622000	-0.029546000
Cl	-3.600443000	-1.691426000	0.001442000
Cl	-3.481536000	1.833725000	0.067857000
N	-0.939162000	-1.098501000	-0.016359000
N	-0.866214000	1.063988000	0.024306000
C	-0.069000000	-0.045215000	-0.005720000
C	-2.207479000	0.711702000	0.032302000
C	-2.253670000	-0.657218000	0.006500000
Cl	4.264822000	-0.189274000	-0.055958000
C	-0.370664000	2.433067000	0.045498000
H	-0.708457000	2.946711000	0.955203000
H	0.724288000	2.383731000	0.032324000
H	-0.728458000	2.981673000	-0.835693000
C	-0.536935000	-2.497647000	-0.047989000
H	-0.929698000	-2.986927000	-0.949012000
H	0.558870000	-2.521662000	-0.060648000
H	-0.909736000	-3.021699000	0.841897000

[NHC(Ph)→AgCl]

E= -2213.64405212

Ag	6.448751000	2.359321000	7.530010000
Cl	5.283355000	6.521150000	3.632300000
Cl	5.125747000	7.977419000	6.783949000
N	5.794961000	4.436110000	5.341130000

N	5.696636000	5.345355000	7.308857000
C	5.938429000	4.155064000	6.674546000
C	5.404248000	6.350888000	6.387598000
C	5.466312000	5.777609000	5.146862000
Cl	7.080581000	0.372769000	8.479892000
C	5.725498000	5.507236000	8.735614000
C	4.587571000	5.964982000	9.403660000
C	6.887970000	5.176745000	9.435074000
C	4.620932000	6.098275000	10.791768000
C	6.905811000	5.303919000	10.824378000
C	5.776828000	5.767461000	11.502797000
H	3.681090000	6.197611000	8.844081000
H	7.762224000	4.815448000	8.893184000
H	3.732792000	6.448418000	11.319608000
H	7.807919000	5.035942000	11.375603000
H	5.795098000	5.864590000	12.589264000
C	5.947164000	3.457948000	4.300596000
C	7.149749000	2.755984000	4.196521000
C	4.886282000	3.204112000	3.428361000
C	7.286595000	1.783338000	3.205615000
C	5.038719000	2.236936000	2.434855000
C	6.235713000	1.525745000	2.322993000
H	7.962045000	2.966495000	4.892481000
H	3.946397000	3.745963000	3.537744000
H	8.220089000	1.224728000	3.128136000
H	4.210981000	2.029304000	1.755335000
H	6.346937000	0.763775000	1.550201000

[NHC(Si(CH3)3)→AgCl]

E= -2568.8370226

Ag	6.576857000	2.516912000	7.656091000
Cl	4.979526000	6.426956000	3.612485000
Cl	4.724334000	7.928577000	6.630674000
N	5.772945000	4.416224000	5.325919000
N	5.608762000	5.392573000	7.310173000
C	5.944106000	4.216752000	6.675079000
C	5.227998000	6.324419000	6.348878000
C	5.329605000	5.721946000	5.127477000
Si	6.067094000	3.193810000	3.969177000
Si	5.717303000	5.504515000	9.160022000
C	6.656384000	1.559252000	4.646484000
H	5.930850000	1.069000000	5.309751000
H	6.804023000	0.901076000	3.772395000
H	7.615726000	1.622040000	5.177895000
C	7.394559000	3.934559000	2.871881000
H	8.317118000	4.105493000	3.446168000
H	7.632677000	3.221646000	2.067294000
H	7.095703000	4.882513000	2.407075000
C	4.419659000	2.959493000	3.105492000
H	4.535893000	2.206026000	2.311101000
H	3.665361000	2.582059000	3.811694000
H	4.034612000	3.878873000	2.646716000
C	7.506910000	5.222157000	9.628766000
H	7.622041000	5.406171000	10.708764000
H	7.843832000	4.195869000	9.425042000
H	8.169151000	5.920087000	9.095532000

C	5.203006000	7.214928000	9.732244000
H	4.162324000	7.462430000	9.486468000
H	5.292660000	7.205610000	10.831108000
H	5.851834000	8.015016000	9.353333000
C	4.523304000	4.246522000	9.862828000
H	3.510354000	4.396789000	9.461113000
H	4.829050000	3.210080000	9.661346000
H	4.475771000	4.377162000	10.955611000
Cl	7.274753000	0.659250000	8.817914000

[NHC(SiH3)→AgCl]

E= -2333.108432

Ag	5.891696000	2.274321000	7.578685000
Cl	5.938642000	6.523319000	3.628584000
Cl	5.852724000	8.025178000	6.814050000
N	5.920203000	4.414141000	5.358272000
N	5.866727000	5.348733000	7.340540000
C	5.892757000	4.130977000	6.703211000
C	5.877932000	6.376151000	6.398919000
C	5.911214000	5.794302000	5.164821000
Cl	5.890835000	0.205364000	8.554317000
Si	5.824447000	5.553200000	9.136787000
H	5.825721000	4.170929000	9.676195000
H	7.034270000	6.332394000	9.517854000
H	4.583928000	6.308747000	9.462819000
Si	5.960973000	3.158328000	4.057745000
H	5.956797000	1.862747000	4.780987000
H	4.752011000	3.362322000	3.213448000

H	7.202356000	3.385183000	3.268106000

[NHC(H)→AgCl]

E= -1751.9897221

Ag	5.900801000	2.283259000	7.649548000
Cl	5.964701000	6.436633000	3.609227000
Cl	5.799364000	8.015720000	6.806794000
N	5.940249000	4.403782000	5.416417000
N	5.841780000	5.345420000	7.323125000
C	5.893860000	4.112783000	6.746171000
C	5.854717000	6.373665000	6.392009000
C	5.918146000	5.767973000	5.165552000
Cl	5.908328000	0.237824000	8.658896000
H	5.985936000	3.691717000	4.694672000
H	5.798325000	5.485698000	8.327354000

[NHC(C(CH3)3)→AgCl]

E=-2066.1289255

Cl	5.890771000	6.557481000	3.664343000
Cl	5.629448000	7.978756000	6.611641000
N	5.939150000	4.326305000	5.347806000
N	5.764022000	5.278555000	7.322460000
C	5.817671000	4.058391000	6.690929000
C	5.782981000	6.293769000	6.371119000
C	5.891822000	5.701870000	5.143712000
Cl	4.188105000	0.332828000	8.342701000
C	6.169451000	3.314181000	4.237226000
C	4.952495000	3.327061000	3.299261000

H	4.796703000	4.300563000	2.820120000
H	5.102057000	2.579893000	2.507557000
H	4.043099000	3.055799000	3.853388000
C	7.475933000	3.687024000	3.511028000
H	8.321732000	3.663009000	4.212805000
H	7.665785000	2.940643000	2.727865000
H	7.443858000	4.670989000	3.032866000
C	6.350410000	1.896461000	4.781753000
H	6.615644000	1.256361000	3.927918000
H	7.160944000	1.830845000	5.518987000
H	5.432691000	1.484230000	5.225352000
C	5.762955000	5.525326000	8.822419000
C	5.921671000	4.228245000	9.617141000
H	6.017298000	4.510268000	10.675641000
H	6.822784000	3.669853000	9.332601000
C	4.428308000	6.178884000	9.212905000
H	4.273081000	7.149111000	8.726990000
H	3.590885000	5.515792000	8.954699000
H	4.411443000	6.337933000	10.300028000
C	6.974852000	6.412999000	9.163934000
H	6.999062000	6.568344000	10.251017000
H	7.908537000	5.910651000	8.873544000
H	6.942602000	7.397661000	8.687219000
Ag	5.133608000	2.254782000	7.499943000
H	5.050566000	3.562426000	9.534739000

[{$(Ph)_3$PCHBr}→CuCl]

E=-5748.317247

C	-0.402069000	-0.515901000	-1.393088000
P	0.508551000	0.169734000	-0.019911000
C	-0.070169000	1.883337000	0.172987000
C	0.283610000	2.818061000	-0.815458000
C	-0.891807000	2.273385000	1.239956000
C	-0.199359000	4.123581000	-0.742767000
C	-1.361883000	3.584850000	1.310247000
C	-1.022228000	4.507748000	0.319338000
H	0.935890000	2.527087000	-1.641374000
H	-1.174763000	1.553062000	2.007611000
H	0.068587000	4.842987000	-1.518185000
H	-2.007451000	3.880810000	2.138237000
H	-1.400904000	5.529784000	0.372853000
C	0.218702000	-0.781291000	1.501923000
C	-1.090346000	-1.125749000	1.881948000
C	1.300899000	-1.185852000	2.299569000
C	-1.306171000	-1.861222000	3.046574000
C	1.074792000	-1.923414000	3.462403000
C	-0.226768000	-2.260630000	3.838250000
H	-1.944529000	-0.829546000	1.261379000
H	2.321659000	-0.937197000	2.008719000
H	-2.326702000	-2.125471000	3.327880000
H	1.922609000	-2.240130000	4.072033000
H	-0.400016000	-2.840695000	4.746549000
C	2.320022000	0.327780000	-0.228712000
C	2.999480000	-0.437199000	-1.189179000

C	3.037498000	1.250013000	0.553695000
C	4.377286000	-0.282906000	-1.358439000
C	4.413936000	1.395613000	0.382031000
C	5.085818000	0.629172000	-0.574242000
H	2.452989000	-1.159768000	-1.796900000
H	2.518075000	1.863763000	1.292171000
H	4.896665000	-0.881010000	-2.108993000
H	4.961544000	2.115550000	0.992624000
H	6.162318000	0.747088000	-0.710144000
Cu	-2.251847000	-0.209843000	-0.998528000
Cl	-4.252949000	0.158293000	-0.420004000
Br	0.052428000	-2.448816000	-1.656349000
H	-0.092985000	-0.005543000	-2.318404000

[{$(Ph)_3$PCHCF3}→CuCl]

E= -3512.027806

C	-0.381090000	0.000464000	-1.980088000
P	0.497928000	-0.083217000	-0.427560000
C	0.215385000	1.499370000	0.432129000
C	1.271499000	2.378572000	0.715504000
C	-1.093591000	1.831823000	0.825855000
C	1.017420000	3.588877000	1.364378000
C	-1.336749000	3.045280000	1.468712000
C	-0.285181000	3.925626000	1.736148000
H	2.293655000	2.121322000	0.436783000
H	-1.926781000	1.148576000	0.626908000
H	1.844117000	4.267994000	1.579218000
H	-2.356926000	3.296951000	1.762417000

H	-0.481233000	4.873313000	2.241014000
C	-0.081959000	-1.389950000	0.694606000
C	-0.828979000	-2.484054000	0.235847000
C	0.220873000	-1.276641000	2.062195000
C	-1.262191000	-3.456503000	1.137435000
C	-0.217326000	-2.252682000	2.957387000
C	-0.958395000	-3.343096000	2.495349000
H	-1.092444000	-2.568252000	-0.818421000
H	0.781850000	-0.416220000	2.432425000
H	-1.854867000	-4.296996000	0.774215000
H	0.009734000	-2.151974000	4.019875000
H	-1.310556000	-4.099860000	3.198428000
C	2.305770000	-0.297704000	-0.599380000
C	3.000146000	0.535199000	-1.494624000
C	3.007421000	-1.287476000	0.104157000
C	4.376364000	0.392180000	-1.662925000
C	4.384888000	-1.430646000	-0.074170000
C	5.071114000	-0.589884000	-0.951675000
H	2.461705000	1.285938000	-2.075240000
H	2.478236000	-1.953796000	0.785798000
H	4.905231000	1.042567000	-2.361424000
H	4.920969000	-2.207418000	0.473560000
H	6.147357000	-0.705664000	-1.090686000
Cu	-2.244028000	-0.207350000	-1.411898000
Cl	-4.216310000	-0.323732000	-0.661492000
H	-0.324133000	1.045746000	-2.325027000
C	0.074538000	-0.901074000	-3.093723000
F	-0.864045000	-1.023128000	-4.068807000

F	0.371669000	-2.167517000	-2.661575000
F	1.206813000	-0.454139000	-3.737995000

[{$(Ph)_3$PCHCl}→CuCl]

E= -3634.571424

C	-0.390804000	-0.160694000	-1.699714000
P	0.511945000	0.012761000	-0.165599000
C	-0.077097000	1.554581000	0.595310000
C	0.345257000	2.774231000	0.039101000
C	-0.985548000	1.552583000	1.663732000
C	-0.153683000	3.976706000	0.538749000
C	-1.470836000	2.760441000	2.164222000
C	-1.061477000	3.970686000	1.600540000
H	1.063407000	2.785723000	-0.783025000
H	-1.323935000	0.611706000	2.097586000
H	0.168381000	4.920665000	0.096182000
H	-2.184086000	2.752006000	2.989399000
H	-1.452758000	4.912771000	1.988193000
C	0.232479000	-1.416975000	0.923663000
C	-1.068617000	-1.903789000	1.139920000
C	1.319947000	-2.050823000	1.546437000
C	-1.271549000	-3.003360000	1.973178000
C	1.107018000	-3.151757000	2.376861000
C	-0.187192000	-3.628298000	2.593204000
H	-1.927562000	-1.431418000	0.648073000
H	2.336018000	-1.694780000	1.376280000
H	-2.286431000	-3.372269000	2.129347000
H	1.959631000	-3.640976000	2.850664000
H	-0.350516000	-4.491701000	3.240787000

C	2.323756000	0.231981000	-0.304666000
C	2.999063000	-0.170003000	-1.467894000
C	3.045052000	0.834880000	0.741039000
C	4.377660000	0.026229000	-1.577330000
C	4.422212000	1.024101000	0.625702000
C	5.090059000	0.619572000	-0.533520000
H	2.448261000	-0.642146000	-2.282515000
H	2.527143000	1.167034000	1.642866000
H	4.895055000	-0.287291000	-2.485528000
H	4.973589000	1.495216000	1.441252000
H	6.167098000	0.771633000	-0.623637000
Cu	-2.243568000	-0.016247000	-1.201061000
Cl	-4.243176000	0.102775000	-0.517197000
H	-0.110408000	0.674861000	-2.361244000
Cl	0.061247000	-1.708248000	-2.558163000

[{$(Ph)_3$PCHF}→CuCl]

E= -3274.326603

C	-0.374836000	0.111169000	-1.908565000
P	0.521336000	-0.011211000	-0.341720000
C	0.272457000	1.551476000	0.540425000
C	1.328535000	2.466698000	0.676694000
C	-1.006344000	1.875301000	1.029808000
C	1.104521000	3.700785000	1.288422000
C	-1.219182000	3.115086000	1.633990000
C	-0.168665000	4.026715000	1.762417000
H	2.323608000	2.215529000	0.306736000
H	-1.838881000	1.173363000	0.923747000

H	1.927761000	4.409611000	1.390986000
H	-2.216237000	3.364816000	1.999600000
H	-0.341939000	4.994874000	2.235912000
C	-0.097365000	-1.385127000	0.662241000
C	-0.580287000	-2.539657000	0.023446000
C	-0.071654000	-1.316697000	2.063378000
C	-1.032556000	-3.612909000	0.788815000
C	-0.530731000	-2.396398000	2.820579000
C	-1.009276000	-3.543145000	2.184810000
H	-0.615290000	-2.588839000	-1.065790000
H	0.283953000	-0.414013000	2.563526000
H	-1.418102000	-4.503680000	0.290788000
H	-0.523419000	-2.334399000	3.909983000
H	-1.375780000	-4.382378000	2.778389000
C	2.318795000	-0.273422000	-0.543994000
C	2.940344000	0.231753000	-1.697259000
C	3.082069000	-0.971545000	0.404463000
C	4.311539000	0.056221000	-1.888042000
C	4.453131000	-1.142014000	0.209439000
C	5.069011000	-0.627294000	-0.934336000
H	2.348640000	0.751046000	-2.452964000
H	2.603488000	-1.390882000	1.290881000
H	4.786434000	0.446671000	-2.789562000
H	5.041193000	-1.684899000	0.951345000
H	6.140474000	-0.767923000	-1.087129000
Cu	-2.223618000	0.135898000	-1.379143000
Cl	-4.207351000	0.220193000	-0.640333000
H	-0.069979000	1.063559000	-2.380845000

F	0.053554000	-0.947163000	-2.772518000

[{(Ph)$_3$PCHH}→CuCl]

E= -3175.147303

C	-0.376434000	0.056725000	-1.945327000
P	0.484941000	-0.003526000	-0.411515000
C	0.266320000	1.550578000	0.508843000
C	1.357454000	2.387347000	0.788077000
C	-1.025410000	1.927954000	0.917182000
C	1.157346000	3.595995000	1.458984000
C	-1.214704000	3.136253000	1.587185000
C	-0.126917000	3.971347000	1.857296000
H	2.363587000	2.099793000	0.480093000
H	-1.886570000	1.287350000	0.696684000
H	2.009758000	4.244724000	1.667409000
H	-2.221549000	3.423863000	1.893822000
H	-0.281550000	4.917254000	2.379785000
C	-0.105120000	-1.366993000	0.633218000
C	-0.618069000	-2.528242000	0.034893000
C	-0.028315000	-1.280661000	2.031322000
C	-1.040739000	-3.592449000	0.829440000
C	-0.459371000	-2.348384000	2.821595000
C	-0.962130000	-3.504219000	2.222227000
H	-0.714858000	-2.589795000	-1.049946000
H	0.343525000	-0.369980000	2.504680000
H	-1.450363000	-4.487325000	0.358747000
H	-0.412430000	-2.269352000	3.908963000
H	-1.307356000	-4.333946000	2.841340000

H	-0.106183000	-0.808187000	-2.571928000
C	2.296659000	-0.253462000	-0.576594000
C	2.924867000	0.213595000	-1.741909000
C	3.064720000	-0.899369000	0.404688000
C	4.299751000	0.048746000	-1.917305000
C	4.438774000	-1.065716000	0.224257000
C	5.058369000	-0.590637000	-0.934342000
H	2.332469000	0.700750000	-2.518894000
H	2.587551000	-1.285878000	1.306571000
H	4.777190000	0.414838000	-2.827844000
H	5.026515000	-1.574334000	0.990453000
H	6.132300000	-0.725677000	-1.074356000
Cu	-2.250366000	0.061374000	-1.447663000
Cl	-4.266841000	0.111072000	-0.799234000
H	-0.111549000	0.990277000	-2.466001000

[{(Ph)$_3$PCHMe}→CuCl]

E= -3214.409908

C	-0.062739000	-0.350856000	-1.859826000
P	0.535590000	0.010380000	-0.236592000
C	-0.126799000	1.593092000	0.381616000
C	-1.111666000	2.298969000	-0.324245000
C	0.371929000	2.118680000	1.584564000
C	-1.591847000	3.512658000	0.170505000
C	-0.120794000	3.325288000	2.080578000
C	-1.102379000	4.024514000	1.373448000
H	-1.529952000	1.880521000	-1.243492000
H	1.148824000	1.588719000	2.137911000

H	-2.362636000	4.049714000	-0.384194000
H	0.265459000	3.720723000	3.021475000
H	-1.487501000	4.968577000	1.763063000
C	0.104997000	-1.323332000	0.922857000
C	-1.090463000	-1.247667000	1.655838000
C	0.897764000	-2.479636000	1.002193000
C	-1.478428000	-2.313509000	2.466654000
C	0.497918000	-3.546176000	1.810252000
C	-0.686759000	-3.462370000	2.544316000
H	-1.731868000	-0.369115000	1.571110000
H	1.825149000	-2.552975000	0.431871000
H	-2.414068000	-2.250348000	3.023725000
H	1.113384000	-4.445983000	1.860568000
H	-0.998487000	-4.298080000	3.173335000
C	2.361894000	0.210004000	-0.107088000
C	3.036865000	0.710564000	-1.231316000
C	3.093422000	-0.073685000	1.057478000
C	4.414489000	0.929586000	-1.191080000
C	4.471411000	0.146928000	1.095682000
C	5.133749000	0.648371000	-0.027318000
H	2.478770000	0.930961000	-2.144035000
H	2.588016000	-0.476363000	1.936831000
H	4.927486000	1.317366000	-2.072830000
H	5.029661000	-0.076622000	2.006637000
H	6.211647000	0.816544000	0.003657000
Cu	-1.973110000	-0.519768000	-1.461825000
Cl	-4.036462000	-0.675928000	-1.009197000
H	0.078310000	0.552433000	-2.479414000

C	0.556365000	-1.596753000	-2.512252000
H	1.646135000	-1.516862000	-2.676936000
H	0.375084000	-2.500342000	-1.912456000
H	0.085452000	-1.767413000	-3.489856000

[{(Ph)$_3$PCHPh}→CuCl]

E= -3405.974198

C	-0.089691000	-0.477645000	-1.783339000
P	0.553311000	-0.081823000	-0.175403000
C	-0.181213000	1.500155000	0.373925000
C	-1.290333000	2.061178000	-0.276323000
C	0.381170000	2.170160000	1.473121000
C	-1.825515000	3.271597000	0.166789000
C	-0.163323000	3.374831000	1.917111000
C	-1.266977000	3.928829000	1.264052000
H	-1.760196000	1.534066000	-1.110827000
H	1.251151000	1.758245000	1.985691000
H	-2.691733000	3.692325000	-0.345972000
H	0.279679000	3.882401000	2.775601000
H	-1.692778000	4.871118000	1.613444000
C	0.211494000	-1.339784000	1.097205000
C	-1.023742000	-1.311079000	1.765256000
C	1.120231000	-2.377416000	1.360305000
C	-1.338304000	-2.305014000	2.691125000
C	0.795979000	-3.370610000	2.286555000
C	-0.430016000	-3.333396000	2.954075000
H	-1.753983000	-0.531695000	1.540970000
H	2.074431000	-2.422981000	0.834096000

H	-2.305503000	-2.280714000	3.194647000
H	1.503474000	-4.178588000	2.480507000
H	-0.682013000	-4.112905000	3.675307000
C	2.367093000	0.194973000	-0.131325000
C	2.997033000	0.544781000	-1.335550000
C	3.132692000	0.122946000	1.045502000
C	4.363996000	0.825294000	-1.362566000
C	4.498704000	0.406502000	1.014616000
C	5.115968000	0.758987000	-0.188261000
H	2.417511000	0.581820000	-2.258588000
H	2.666503000	-0.164898000	1.989137000
H	4.842497000	1.089293000	-2.307033000
H	5.083499000	0.347988000	1.934327000
H	6.185444000	0.975469000	-0.210313000
Cu	-1.959746000	-0.877971000	-1.338916000
Cl	-3.972271000	-1.228988000	-0.784701000
H	-0.094744000	0.472237000	-2.345648000
C	0.553230000	-1.567227000	-2.586053000
C	0.678921000	-2.892650000	-2.125973000
C	1.016706000	-1.285069000	-3.885460000
C	1.264228000	-3.878246000	-2.920395000
C	1.588565000	-2.274791000	-4.685917000
C	1.726003000	-3.578018000	-4.204731000
H	0.281590000	-3.162948000	-1.146313000
H	0.910676000	-0.270179000	-4.279057000
H	1.342823000	-4.897706000	-2.536946000
H	1.927516000	-2.023298000	-5.693077000
H	2.172450000	-4.354344000	-4.827984000

[{(Ph)$_3$PCHSi(CH3)3}→CuCl]

E= -3583.555616

C	0.517471000	-0.706939000	-1.167320000
P	-0.597130000	0.118820000	-0.107321000
C	-0.288141000	-0.273528000	1.642135000
C	-1.146755000	-1.129744000	2.347709000
C	0.860099000	0.237978000	2.271448000
C	-0.856583000	-1.476516000	3.669189000
C	1.138820000	-0.109000000	3.593357000
C	0.284116000	-0.966076000	4.292173000
H	-2.040704000	-1.528613000	1.865964000
H	1.549241000	0.887311000	1.722468000
H	-1.524859000	-2.148213000	4.210600000
H	2.035030000	0.287516000	4.072923000
H	0.509345000	-1.238467000	5.324966000
C	-0.520518000	1.936237000	-0.279527000
C	-0.226075000	2.493104000	-1.534086000
C	-0.799468000	2.783619000	0.802970000
C	-0.210369000	3.876493000	-1.700117000
C	-0.772623000	4.169654000	0.632832000
C	-0.480947000	4.717327000	-0.616873000
H	0.018103000	1.845549000	-2.377846000
H	-1.009412000	2.365644000	1.788890000
H	0.030795000	4.299800000	-2.676369000
H	-0.970596000	4.821761000	1.485238000
H	-0.452527000	5.800547000	-0.745975000

H	0.235380000	-0.507763000	-2.217120000
C	-2.373866000	-0.248357000	-0.413755000
C	-2.718601000	-1.196431000	-1.384788000
C	-3.394195000	0.438561000	0.266183000
C	-4.060582000	-1.463859000	-1.668528000
C	-4.732334000	0.167088000	-0.014936000
C	-5.068167000	-0.784615000	-0.983175000
H	-1.929994000	-1.727748000	-1.918070000
H	-3.146262000	1.194334000	1.013407000
H	-4.315704000	-2.205172000	-2.427807000
H	-5.517364000	0.705435000	0.519107000
H	-6.116669000	-0.991471000	-1.204790000
Si	1.109472000	-2.499911000	-0.978293000
C	2.247503000	-2.802922000	-2.453746000
H	3.133429000	-2.152623000	-2.408240000
H	2.591366000	-3.848740000	-2.467876000
H	1.734261000	-2.607043000	-3.407575000
C	2.059153000	-2.795963000	0.623867000
H	1.418460000	-2.716458000	1.513468000
H	2.480265000	-3.813998000	0.607079000
H	2.890654000	-2.084879000	0.737031000
C	-0.279107000	-3.793413000	-1.051837000
H	0.150716000	-4.799533000	-0.923141000
H	-1.026017000	-3.649138000	-0.256928000
H	-0.805784000	-3.785787000	-2.018244000
Cu	2.147362000	0.310683000	-0.765713000
Cl	3.891572000	1.374601000	-0.208153000

[{(Ph)$_3$PCHSiH3}→CuCl]

E= -3465.699429

C	0.353884000	-0.500687000	-1.666978000
P	-0.502313000	0.025875000	-0.233053000
C	-0.287606000	-1.156446000	1.132044000
C	-1.370380000	-1.915192000	1.600597000
C	0.988420000	-1.337568000	1.694481000
C	-1.177169000	-2.855164000	2.615236000
C	1.170992000	-2.278272000	2.707581000
C	0.091649000	-3.037814000	3.167752000
H	-2.364302000	-1.776036000	1.173273000
H	1.843950000	-0.759098000	1.329980000
H	-2.022649000	-3.445951000	2.971437000
H	2.165784000	-2.418331000	3.133255000
H	0.241197000	-3.774464000	3.959300000
C	0.063897000	1.654360000	0.357892000
C	0.518098000	2.604729000	-0.569675000
C	0.019282000	1.982788000	1.721037000
C	0.917058000	3.867958000	-0.137245000
C	0.428237000	3.248015000	2.149006000
C	0.874008000	4.191073000	1.221917000
H	0.586740000	2.349585000	-1.628428000
H	-0.311622000	1.243558000	2.452709000
H	1.279870000	4.596924000	-0.863373000
H	0.407971000	3.490680000	3.212757000
H	1.201680000	5.175887000	1.558990000
H	0.095973000	0.149223000	-2.520003000
C	-2.308779000	0.224396000	-0.483670000

C	-2.943122000	-0.529397000	-1.483655000
C	-3.069021000	1.114287000	0.292520000
C	-4.317583000	-0.401814000	-1.695295000
C	-4.441756000	1.238372000	0.076706000
C	-5.068413000	0.480338000	-0.915723000
H	-2.360455000	-1.217795000	-2.098109000
H	-2.587013000	1.723725000	1.058444000
H	-4.800275000	-0.992475000	-2.475765000
H	-5.022650000	1.936146000	0.682362000
H	-6.141706000	0.582624000	-1.085489000
Si	0.406692000	-2.309264000	-2.157500000
H	1.328638000	-2.458936000	-3.323735000
H	0.868284000	-3.166676000	-1.025483000
H	-0.924773000	-2.866607000	-2.601701000
Cu	2.219136000	-0.235584000	-1.144209000
Cl	4.197132000	0.049281000	-0.454984000

[{$(Ph)_3$PCHC(CH3)3}→CuCl]

E= -3332.213875

C	-0.419908000	-0.929115000	-1.217547000
P	0.487047000	0.073298000	-0.066288000
C	-0.052634000	1.796331000	-0.348440000
C	-0.228416000	2.292717000	-1.652791000
C	-0.267027000	2.652591000	0.742114000
C	-0.620502000	3.614710000	-1.854850000
C	-0.663953000	3.974345000	0.532572000
C	-0.841620000	4.458782000	-0.763263000
H	-0.070096000	1.647581000	-2.517992000

H	-0.146427000	2.282756000	1.760750000
H	-0.762828000	3.983624000	-2.871873000
H	-0.843874000	4.623472000	1.391021000
H	-1.159148000	5.490169000	-0.924804000
C	0.218035000	-0.291881000	1.708558000
C	-1.007912000	-0.802895000	2.161049000
C	1.211064000	0.028671000	2.652010000
C	-1.229188000	-1.008258000	3.522837000
C	0.984169000	-0.176336000	4.013798000
C	-0.233860000	-0.700501000	4.452160000
H	-1.810483000	-1.015872000	1.444906000
H	2.165166000	0.443976000	2.327213000
H	-2.191524000	-1.403019000	3.852483000
H	1.764610000	0.077742000	4.733139000
H	-0.409083000	-0.861193000	5.517588000
C	2.327842000	0.114272000	-0.231517000
C	3.109182000	-0.952569000	0.248642000
C	2.963611000	1.152151000	-0.930241000
C	4.486928000	-0.977564000	0.036156000
C	4.343757000	1.122858000	-1.145642000
C	5.108682000	0.059640000	-0.664771000
H	2.641180000	-1.768756000	0.802001000
H	2.382212000	1.996996000	-1.301194000
H	5.076969000	-1.811973000	0.419537000
H	4.821332000	1.941507000	-1.687008000
H	6.187098000	0.039368000	-0.830821000
Cu	-2.248798000	-0.446818000	-0.693075000
Cl	-4.262700000	-0.044205000	-0.169606000

H	-0.327341000	-0.364707000	-2.166037000
C	-0.123396000	-2.427645000	-1.505933000
C	-0.057084000	-3.268894000	-0.223411000
H	0.766372000	-2.960624000	0.438623000
H	-0.993713000	-3.191776000	0.346757000
H	0.102542000	-4.328590000	-0.474604000
C	1.178088000	-2.603312000	-2.314899000
H	2.066737000	-2.276916000	-1.758362000
H	1.322905000	-3.661207000	-2.585500000
H	1.135747000	-2.024073000	-3.250452000
C	-1.286385000	-2.957109000	-2.369398000
H	-1.113456000	-4.010909000	-2.640740000
H	-2.243205000	-2.884984000	-1.830343000
H	-1.383183000	-2.378753000	-3.300648000

[{(Ph)$_3$PCHCBr}→AuCl]

E= -4243.80723

C	0.144009000	0.047467000	-1.871815000
P	-0.763186000	-0.027365000	-0.314975000
C	-0.178658000	-1.340930000	0.787565000
C	0.476040000	-2.477152000	0.287675000
C	-0.408803000	-1.215014000	2.167648000
C	0.892793000	-3.475890000	1.167515000
C	0.010372000	-2.221016000	3.039040000
C	0.660874000	-3.351172000	2.539399000
H	0.671166000	-2.573961000	-0.780331000
H	-0.896873000	-0.323136000	2.565109000
H	1.413322000	-4.350917000	0.775969000

H	-0.161032000	-2.113190000	4.111193000
H	0.997587000	-4.132827000	3.222596000
C	-0.535588000	1.559067000	0.546987000
C	0.743835000	1.905159000	1.017736000
C	-1.610015000	2.443086000	0.733803000
C	0.940578000	3.131268000	1.651470000
C	-1.402504000	3.667098000	1.372213000
C	-0.128813000	4.013386000	1.827397000
H	1.584435000	1.223308000	0.869672000
H	-2.608954000	2.176396000	0.387752000
H	1.938242000	3.396145000	2.004557000
H	-2.241767000	4.350064000	1.513264000
H	0.031047000	4.972353000	2.323570000
H	-0.179484000	0.966771000	-2.382357000
C	-2.555374000	-0.258201000	-0.560516000
C	-3.194139000	0.468583000	-1.580081000
C	-3.301091000	-1.150507000	0.222188000
C	-4.562845000	0.317306000	-1.796043000
C	-4.671231000	-1.300721000	-0.001650000
C	-5.303497000	-0.565939000	-1.005821000
H	-2.620225000	1.145782000	-2.215295000
H	-2.811279000	-1.737581000	0.999855000
H	-5.049718000	0.882707000	-2.592136000
H	-5.243651000	-2.000445000	0.609408000
H	-6.373731000	-0.687987000	-1.181028000
Au	2.152392000	0.062673000	-1.528673000
Cl	4.412783000	0.133547000	-1.168372000
Br	-0.505432000	-1.423469000	-3.080499000

[{(Ph)$_3$PCHC (CH3)3}→AuCl]

E= -1827.701944

C	0.175743000	-0.719556000	-1.203282000
P	-0.964088000	-0.000805000	-0.015990000
C	-0.807185000	-0.724003000	1.646359000
C	-1.635193000	-1.780557000	2.057482000
C	0.223907000	-0.283208000	2.491317000
C	-1.437751000	-2.382867000	3.300994000
C	0.413692000	-0.887845000	3.733948000
C	-0.415131000	-1.936136000	4.140661000
H	-2.427242000	-2.147454000	1.403532000
H	0.895328000	0.513209000	2.164751000
H	-2.081448000	-3.208519000	3.608730000
H	1.223598000	-0.543261000	4.378433000
H	-0.259513000	-2.410788000	5.111122000
C	-0.699868000	1.801612000	0.109884000
C	-0.095967000	2.525184000	-0.928987000
C	-1.207162000	2.484960000	1.224907000
C	0.002497000	3.913669000	-0.845526000
C	-1.091975000	3.873401000	1.308991000
C	-0.489723000	4.589681000	0.273441000
H	0.329062000	2.006353000	-1.788150000
H	-1.679664000	1.935170000	2.040593000
H	0.484760000	4.466494000	-1.652981000
H	-1.472151000	4.393763000	2.189602000
H	-0.397016000	5.674917000	0.340963000
H	-0.012380000	-0.160875000	-2.140110000

C	-2.760346000	-0.037080000	-0.447956000
C	-3.113919000	0.010385000	-1.805317000
C	-3.776190000	0.039244000	0.519162000
C	-4.451848000	0.105664000	-2.188625000
C	-5.114671000	0.129360000	0.133426000
C	-5.456280000	0.158823000	-1.220117000
H	-2.338578000	-0.024510000	-2.572069000
H	-3.528154000	0.030357000	1.581112000
H	-4.709046000	0.137771000	-3.248729000
H	-5.892991000	0.181262000	0.896863000
H	-6.503296000	0.229056000	-1.519706000
Au	1.998360000	0.006138000	-0.443544000
Cl	4.029003000	0.748889000	0.343210000
C	0.177401000	-2.249575000	-1.536899000
C	1.109999000	-2.414411000	-2.753228000
H	2.124546000	-2.063642000	-2.515950000
H	1.164799000	-3.473523000	-3.048357000
H	0.744757000	-1.839409000	-3.618844000
C	0.739484000	-3.102345000	-0.386209000
H	0.099105000	-3.076967000	0.505454000
H	0.817723000	-4.152046000	-0.709754000
H	1.739551000	-2.751404000	-0.094621000
C	-1.210487000	-2.794043000	-1.922469000
H	-1.131774000	-3.858685000	-2.191414000
H	-1.933503000	-2.717235000	-1.096812000
H	-1.632774000	-2.266117000	-2.790148000

[{$(Ph)_3$PCHCF3}→AuCl]

E= -2007.51311

C	0.413441000	-0.083921000	-1.725406000
P	-0.697993000	-0.108838000	-0.311807000
C	-0.308548000	-1.463742000	0.825759000
C	-0.910349000	-2.720072000	0.655573000
C	0.670039000	-1.281678000	1.815923000
C	-0.541385000	-3.783033000	1.480183000
C	1.028012000	-2.348812000	2.638690000
C	0.423421000	-3.597341000	2.472613000
H	-1.652007000	-2.875521000	-0.128813000
H	1.168494000	-0.317174000	1.924673000
H	-1.003832000	-4.760980000	1.338504000
H	1.795047000	-2.204569000	3.400632000
H	0.712591000	-4.431973000	3.113667000
C	-0.587480000	1.482448000	0.563602000
C	-0.023013000	2.617046000	-0.036505000
C	-1.165217000	1.583892000	1.838751000
C	-0.036629000	3.838416000	0.637171000
C	-1.163132000	2.805768000	2.511456000
C	-0.601969000	3.934508000	1.910319000
H	0.458692000	2.545548000	-1.011464000
H	-1.604076000	0.707009000	2.317674000
H	0.414287000	4.713982000	0.168194000
H	-1.598833000	2.873074000	3.509491000
H	-0.598470000	4.889392000	2.438528000
H	0.142609000	0.774549000	-2.361917000
C	-2.480025000	-0.234658000	-0.726408000
C	-2.926862000	0.262008000	-1.960098000

C	-3.420463000	-0.705194000	0.205240000
C	-4.289082000	0.281046000	-2.259503000
C	-4.781734000	-0.686616000	-0.100196000
C	-5.218270000	-0.193437000	-1.331695000
H	-2.211078000	0.622788000	-2.699036000
H	-3.093778000	-1.095788000	1.170044000
H	-4.623284000	0.663257000	-3.225269000
H	-5.502981000	-1.060578000	0.628398000
H	-6.283294000	-0.181613000	-1.569384000
Au	2.274139000	0.289688000	-0.849400000
Cl	4.306817000	0.724509000	0.103267000
C	0.407249000	-1.311282000	-2.611993000
F	1.211721000	-1.123422000	-3.686820000
F	0.816186000	-2.441118000	-1.981769000
F	-0.840068000	-1.608258000	-3.129607000

[{$(Ph)_3$PCHCl}→AuCl]

E= -2130.062072

C	-0.081024000	0.021423000	-1.911491000
P	-0.831238000	-0.001438000	-0.265386000
C	-0.267289000	-1.391543000	0.749407000
C	0.152777000	-2.593341000	0.157317000
C	-0.281106000	-1.265877000	2.147988000
C	0.554340000	-3.656002000	0.965650000
C	0.122559000	-2.336208000	2.947600000
C	0.539673000	-3.530709000	2.357214000
H	0.180218000	-2.690922000	-0.927981000
H	-0.586739000	-0.326724000	2.612824000

H	0.893462000	-4.583230000	0.501679000
H	0.122174000	-2.229497000	4.033487000
H	0.864625000	-4.363680000	2.983007000
C	-0.387213000	1.542581000	0.583364000
C	0.947325000	1.760287000	0.970985000
C	-1.355479000	2.528656000	0.831648000
C	1.302913000	2.960153000	1.586027000
C	-0.988736000	3.725126000	1.450103000
C	0.338713000	3.942851000	1.824328000
H	1.706656000	1.000150000	0.774619000
H	-2.395397000	2.363594000	0.548072000
H	2.342061000	3.125038000	1.874272000
H	-1.745839000	4.487776000	1.639289000
H	0.622748000	4.880400000	2.305686000
H	-0.339664000	0.993194000	-2.359680000
C	-2.652888000	-0.079168000	-0.336759000
C	-3.320300000	0.631059000	-1.348861000
C	-3.395449000	-0.832895000	0.583541000
C	-4.712263000	0.599268000	-1.424721000
C	-4.788824000	-0.861927000	0.501693000
C	-5.447827000	-0.145341000	-0.498957000
H	-2.751855000	1.199048000	-2.087244000
H	-2.885682000	-1.405798000	1.359171000
H	-5.222857000	1.149292000	-2.216742000
H	-5.359283000	-1.452808000	1.220139000
H	-6.536859000	-0.173855000	-0.564283000
Au	1.947268000	-0.142781000	-1.703853000
Cl	4.223605000	-0.279385000	-1.481095000

Cl	-0.888393000	-1.238046000	-2.967936000

[{(Ph)$_3$PCHF}→AuCl]

E= -1769.818691

C	-0.050453000	0.071989000	-1.880961000
P	-0.816740000	0.041218000	-0.223309000
C	-0.258596000	-1.378560000	0.750208000
C	-0.003889000	-2.598678000	0.101910000
C	-0.120411000	-1.278791000	2.142612000
C	0.389559000	-3.706151000	0.850652000
C	0.276256000	-2.394680000	2.882412000
C	0.530271000	-3.606385000	2.237937000
H	-0.095626000	-2.674086000	-0.982193000
H	-0.302094000	-0.327975000	2.646644000
H	0.600150000	-4.649380000	0.344613000
H	0.396396000	-2.311126000	3.963707000
H	0.849008000	-4.474883000	2.816808000
C	-0.394991000	1.581823000	0.632920000
C	0.935288000	1.826270000	1.019787000
C	-1.383133000	2.550690000	0.870952000
C	1.265224000	3.036456000	1.629731000
C	-1.041301000	3.756746000	1.483918000
C	0.281176000	4.000779000	1.861141000
H	1.709689000	1.081423000	0.823838000
H	-2.417141000	2.361760000	0.580068000
H	2.300435000	3.224333000	1.918056000
H	-1.812461000	4.507008000	1.665542000
H	0.546028000	4.946342000	2.337760000

H	-0.323752000	1.042353000	-2.334418000
C	-2.635338000	-0.070521000	-0.319838000
C	-3.296273000	0.490813000	-1.424480000
C	-3.380953000	-0.710093000	0.682629000
C	-4.687140000	0.424962000	-1.514197000
C	-4.771632000	-0.769844000	0.588369000
C	-5.425547000	-0.202060000	-0.507924000
H	-2.724384000	0.967085000	-2.222133000
H	-2.873784000	-1.170159000	1.532144000
H	-5.193559000	0.857124000	-2.378670000
H	-5.345318000	-1.268336000	1.371435000
H	-6.512960000	-0.256666000	-0.582792000
Au	1.967519000	-0.093999000	-1.651939000
Cl	4.245483000	-0.253984000	-1.413075000
F	-0.684169000	-0.941754000	-2.661458000

[{$(Ph)_3$PCHH}→AuCl]

E= -1670.63725

C	0.066605000	-0.072714000	-1.896169000
P	-0.779402000	-0.005607000	-0.334674000
C	-0.240203000	-1.323381000	0.789688000
C	0.362489000	-2.484134000	0.282872000
C	-0.451691000	-1.191432000	2.170669000
C	0.740850000	-3.505991000	1.153732000
C	-0.067923000	-2.216999000	3.035898000
C	0.526164000	-3.374492000	2.527833000
H	0.571049000	-2.574596000	-0.783653000
H	-0.899403000	-0.280496000	2.572859000

H	1.222704000	-4.400304000	0.756084000
H	-0.222535000	-2.104703000	4.110186000
H	0.835450000	-4.171416000	3.206291000
C	-0.542337000	1.588130000	0.510734000
C	0.758958000	2.084446000	0.699520000
C	-1.640262000	2.309422000	1.007303000
C	0.950596000	3.295824000	1.362869000
C	-1.437740000	3.520635000	1.671851000
C	-0.144352000	4.015753000	1.848144000
H	1.616235000	1.524956000	0.310733000
H	-2.654099000	1.930593000	0.872939000
H	1.964446000	3.675904000	1.497730000
H	-2.296358000	4.077492000	2.050805000
H	0.011231000	4.963948000	2.366084000
H	-0.263586000	0.803013000	-2.478884000
C	-2.584042000	-0.214460000	-0.553364000
C	-3.233261000	0.580218000	-1.515071000
C	-3.322538000	-1.173494000	0.154474000
C	-4.597955000	0.423957000	-1.752387000
C	-4.688837000	-1.330652000	-0.091659000
C	-5.328396000	-0.532766000	-1.041232000
H	-2.669975000	1.323382000	-2.083357000
H	-2.829573000	-1.805301000	0.894350000
H	-5.091398000	1.047376000	-2.499858000
H	-5.252953000	-2.083059000	0.462080000
H	-6.395541000	-0.658005000	-1.232282000
H	-0.277476000	-0.980558000	-2.419478000
Au	2.118348000	-0.068631000	-1.658566000

Cl	4.407503000	-0.068295000	-1.472544000

[{(Ph)$_3$PCHMe}→AuCl]

E= -1709.900185

C	0.124048000	-0.054926000	-1.585464000
P	-0.964735000	-0.011507000	-0.171037000
C	-0.685843000	-1.434082000	0.921713000
C	-1.278869000	-2.674815000	0.638559000
C	0.215095000	-1.320842000	1.992188000
C	-0.975050000	-3.788351000	1.424285000
C	0.506653000	-2.435394000	2.777204000
C	-0.085882000	-3.668652000	2.493960000
H	-1.974629000	-2.776222000	-0.195689000
H	0.704534000	-0.367642000	2.196085000
H	-1.432257000	-4.752123000	1.194446000
H	1.213474000	-2.341230000	3.602655000
H	0.151713000	-4.541038000	3.105271000
C	-0.795827000	1.528564000	0.783153000
C	0.033329000	2.572627000	0.349671000
C	-1.565692000	1.689800000	1.946417000
C	0.087683000	3.763820000	1.075372000
C	-1.497150000	2.877876000	2.673104000
C	-0.672474000	3.917677000	2.236135000
H	0.665566000	2.439883000	-0.529338000
H	-2.217354000	0.885843000	2.293493000
H	0.742095000	4.568101000	0.736147000
H	-2.089691000	2.990372000	3.582448000
H	-0.618101000	4.847113000	2.805664000

H	-0.042666000	0.884268000	-2.142583000
C	-2.745517000	-0.053938000	-0.625329000
C	-3.122585000	0.528704000	-1.845938000
C	-3.739936000	-0.580679000	0.214811000
C	-4.466163000	0.585471000	-2.218237000
C	-5.083153000	-0.521368000	-0.160036000
C	-5.448632000	0.061284000	-1.375774000
H	-2.361909000	0.943205000	-2.510569000
H	-3.467059000	-1.047988000	1.162261000
H	-4.744749000	1.038929000	-3.170930000
H	-5.847015000	-0.934355000	0.501189000
H	-6.499367000	0.104304000	-1.667511000
C	-0.107128000	-1.275135000	-2.491032000
H	0.604069000	-1.239277000	-3.326644000
H	0.078306000	-2.215771000	-1.954211000
H	-1.125702000	-1.317464000	-2.915506000
Au	2.024969000	0.034483000	-0.732495000
Cl	4.151635000	0.116097000	0.136317000

[{(Ph)$_3$PCHPh}→AuCl]

E= -1901.46567

C	0.974105000	-0.263226000	-1.356377000
P	-0.223212000	-0.054995000	-0.021494000
C	-0.259281000	-1.528996000	1.041917000
C	0.256097000	-2.758646000	0.606239000
C	-0.850103000	-1.432052000	2.311458000
C	0.175532000	-3.878289000	1.434759000
C	-0.927364000	-2.556188000	3.134406000

C	-0.415283000	-3.779483000	2.696609000
H	0.753343000	-2.837748000	-0.360520000
H	-1.239541000	-0.474965000	2.663328000
H	0.592794000	-4.827646000	1.096158000
H	-1.378920000	-2.471459000	4.124111000
H	-0.466106000	-4.655880000	3.344986000
C	0.091251000	1.372254000	1.068342000
C	1.344539000	1.497946000	1.691883000
C	-0.918755000	2.305488000	1.351048000
C	1.584919000	2.556232000	2.566582000
C	-0.668844000	3.363326000	2.228015000
C	0.581901000	3.492268000	2.833693000
H	2.134795000	0.770286000	1.476806000
H	-1.901513000	2.210767000	0.889212000
H	2.564035000	2.645846000	3.039751000
H	-1.458495000	4.087160000	2.436416000
H	0.775096000	4.320821000	3.517578000
C	-1.914135000	0.136391000	-0.686805000
C	-2.210986000	1.234620000	-1.517466000
C	-2.894396000	-0.846551000	-0.474034000
C	-3.469724000	1.345272000	-2.108321000
C	-4.150764000	-0.728935000	-1.071161000
C	-4.441402000	0.366297000	-1.886662000
H	-1.458527000	2.000790000	-1.708384000
H	-2.676859000	-1.706365000	0.160647000
H	-3.687760000	2.200452000	-2.750137000
H	-4.904501000	-1.498350000	-0.895472000
H	-5.424630000	0.456612000	-2.351748000

H	0.630231000	-1.191796000	-1.848893000
Au	2.821785000	-0.682859000	-0.495073000
Cl	4.891000000	-1.164088000	0.379718000
C	0.956218000	0.855338000	-2.366177000
C	1.456870000	2.136603000	-2.070654000
C	0.441767000	0.630810000	-3.654961000
H	1.901878000	2.323126000	-1.092097000
H	0.055651000	-0.359388000	-3.909730000
C	1.421429000	3.156520000	-3.021066000
C	0.423624000	1.646141000	-4.613450000
H	1.820219000	4.140927000	-2.768092000
H	0.030677000	1.439754000	-5.611042000
C	0.904118000	2.918250000	-4.298249000
H	0.891651000	3.713727000	-5.045295000

[{$(Ph)_3$PCHSi(CH3)3}→AuCl]

E= -2079.042247

C	0.160830000	-0.723438000	-0.979972000
P	-1.023414000	0.170355000	-0.031184000
C	-0.966963000	-0.297081000	1.724972000
C	-1.933524000	-1.149162000	2.279992000
C	0.108790000	0.142516000	2.514968000
C	-1.824419000	-1.557507000	3.610914000
C	0.209082000	-0.267751000	3.843980000
C	-0.755173000	-1.117070000	4.393412000
H	-2.771230000	-1.499424000	1.675649000
H	0.880304000	0.782688000	2.080256000
H	-2.577383000	-2.224600000	4.033822000

H	1.051834000	0.072620000	4.447462000
H	-0.670586000	-1.439216000	5.432822000
C	-0.809702000	1.981309000	-0.125640000
C	-0.269501000	2.553556000	-1.286690000
C	-1.248791000	2.810857000	0.916370000
C	-0.173799000	3.939458000	-1.402416000
C	-1.141923000	4.198032000	0.798301000
C	-0.608399000	4.763409000	-0.360945000
H	0.106702000	1.916029000	-2.087822000
H	-1.650910000	2.377890000	1.834001000
H	0.259451000	4.375871000	-2.303571000
H	-1.468813000	4.836626000	1.620676000
H	-0.519588000	5.847515000	-0.449008000
H	-0.006631000	-0.483252000	-2.045928000
C	-2.757301000	-0.054933000	-0.594791000
C	-3.013977000	-0.724149000	-1.798624000
C	-3.830712000	0.514014000	0.112276000
C	-4.319166000	-0.831284000	-2.285093000
C	-5.133008000	0.399730000	-0.371358000
C	-5.380042000	-0.272490000	-1.572223000
H	-2.191233000	-1.166517000	-2.360524000
H	-3.652481000	1.051785000	1.044844000
H	-4.503825000	-1.355851000	-3.224038000
H	-5.958332000	0.842913000	0.188593000
H	-6.399867000	-0.357044000	-1.951457000
Au	2.012113000	0.099509000	-0.425725000
Cl	4.058275000	0.967158000	0.150686000
Si	0.405185000	-2.612661000	-0.810615000

C	1.154076000	-3.109886000	0.845114000
H	0.493284000	-2.880031000	1.692915000
H	1.331260000	-4.197339000	0.846496000
H	2.114734000	-2.603373000	1.013683000
C	-1.195235000	-3.612152000	-1.024563000
H	-0.969151000	-4.682791000	-0.896996000
H	-1.962208000	-3.348462000	-0.281218000
H	-1.639158000	-3.489902000	-2.023559000
C	1.564970000	-3.095017000	-2.216804000
H	2.541809000	-2.602786000	-2.109128000
H	1.725457000	-4.184253000	-2.220385000
H	1.150870000	-2.815824000	-3.197645000

[{$(Ph)_3$PCHSiH3}→AuCl]

E= -1961.185751

C	0.251135000	-0.037370000	-1.768168000
P	-0.740870000	-0.022077000	-0.307423000
C	-0.277239000	-1.365216000	0.823148000
C	-0.669277000	-2.684014000	0.541264000
C	0.534433000	-1.102169000	1.936272000
C	-0.247773000	-3.726609000	1.366969000
C	0.948073000	-2.149363000	2.759037000
C	0.559696000	-3.460413000	2.474982000
H	-1.301812000	-2.901453000	-0.321020000
H	0.856241000	-0.082482000	2.150918000
H	-0.547870000	-4.750514000	1.138821000
H	1.587031000	-1.939074000	3.617789000
H	0.891109000	-4.278511000	3.116748000

C	-0.629701000	1.567850000	0.587632000
C	0.492595000	2.399216000	0.452872000
C	-1.684008000	1.962371000	1.429530000
C	0.557589000	3.605247000	1.153049000
C	-1.608675000	3.165121000	2.130806000
C	-0.488598000	3.989286000	1.993293000
H	1.323007000	2.088073000	-0.188724000
H	-2.572005000	1.337437000	1.532093000
H	1.436690000	4.241653000	1.039942000
H	-2.432257000	3.461436000	2.782584000
H	-0.433666000	4.932065000	2.540614000
H	0.019996000	0.876581000	-2.342691000
C	-2.526762000	-0.233365000	-0.654264000
C	-3.042799000	0.290579000	-1.849642000
C	-3.396498000	-0.861539000	0.251694000
C	-4.405516000	0.193902000	-2.130749000
C	-4.759673000	-0.958603000	-0.034730000
C	-5.265731000	-0.430235000	-1.224077000
H	-2.376870000	0.769103000	-2.569616000
H	-3.007607000	-1.283754000	1.179681000
H	-4.794864000	0.601433000	-3.065052000
H	-5.426674000	-1.452099000	0.674223000
H	-6.330925000	-0.509793000	-1.447767000
Au	2.266793000	-0.023071000	-1.213920000
Cl	4.489029000	0.006055000	-0.657320000
Si	0.175224000	-1.541814000	-2.905252000
H	0.708805000	-2.769998000	-2.246127000
H	-1.231172000	-1.863848000	-3.345187000

H	0.961095000	-1.229990000	-4.134734000

[{(Ph)$_3$PCHBr}→AgCl]

E= -3214.409908

C	-2.144409000	0.434013000	-2.095891000
P	-2.998969000	0.873240000	-0.594004000
C	-3.144275000	-0.511902000	0.567119000
C	-3.091436000	-1.840783000	0.119839000
C	-3.316049000	-0.240873000	1.934698000
C	-3.214688000	-2.884807000	1.036560000
C	-3.438898000	-1.291955000	2.844264000
C	-3.389228000	-2.613603000	2.395535000
H	-2.941626000	-2.059093000	-0.937893000
H	-3.332074000	0.790235000	2.293063000
H	-3.160299000	-3.916008000	0.685036000
H	-3.559666000	-1.075641000	3.906915000
H	-3.474851000	-3.434910000	3.109060000
C	-2.011624000	2.167987000	0.214308000
C	-0.760726000	1.831081000	0.762988000
C	-2.454121000	3.499482000	0.254183000
C	0.040021000	2.823987000	1.327064000
C	-1.647024000	4.484779000	0.825338000
C	-0.399806000	4.149592000	1.356803000
H	-0.405683000	0.797878000	0.740802000
H	-3.429287000	3.767760000	-0.153473000
H	1.013374000	2.554572000	1.739360000
H	-1.996556000	5.518103000	0.852984000
H	0.230302000	4.923579000	1.798646000

H	-1.907702000	1.368767000	-2.624084000
C	-4.676862000	1.542175000	-0.863305000
C	-4.885177000	2.390856000	-1.963798000
C	-5.754548000	1.221601000	-0.025578000
C	-6.148687000	2.928679000	-2.205278000
C	-7.018661000	1.759469000	-0.274799000
C	-7.216190000	2.615490000	-1.359801000
H	-4.061386000	2.620451000	-2.642212000
H	-5.610809000	0.542793000	0.815735000
H	-6.302109000	3.583875000	-3.064210000
H	-7.852697000	1.502636000	0.380324000
H	-8.206275000	3.031285000	-1.554447000
Ag	-0.335492000	-0.547000000	-1.618644000
Cl	1.652683000	-1.534719000	-1.006556000
Br	-3.339606000	-0.575211000	-3.323292000

[{$(Ph)_3$PCH(C(CH3)3}→AgCl]

E= -1972.40149

C	0.306560000	-0.735194000	-1.288634000
P	-0.734483000	0.002326000	-0.060451000
C	-0.477922000	-0.707376000	1.596222000
C	-1.312792000	-1.723786000	2.086545000
C	0.636303000	-0.302829000	2.349691000
C	-1.039459000	-2.323479000	3.316958000
C	0.903309000	-0.905925000	3.578995000
C	0.067362000	-1.914655000	4.064060000
H	-2.171209000	-2.060713000	1.504014000
H	1.310036000	0.467641000	1.966684000

H	-1.690040000	-3.117614000	3.686913000
H	1.776965000	-0.590051000	4.150853000
H	0.282443000	-2.387065000	5.024198000
C	-0.408525000	1.798126000	0.037870000
C	0.183511000	2.491985000	-1.027626000
C	-0.839196000	2.507996000	1.168614000
C	0.345586000	3.875515000	-0.957228000
C	-0.662028000	3.890494000	1.239458000
C	-0.072024000	4.576331000	0.176285000
H	0.545791000	1.953596000	-1.903763000
H	-1.299677000	1.982487000	2.006982000
H	0.817414000	4.403585000	-1.787073000
H	-0.983164000	4.430581000	2.131623000
H	0.069847000	5.656769000	0.233908000
H	0.120484000	-0.167020000	-2.218033000
C	-2.559848000	0.004178000	-0.356015000
C	-3.003182000	-0.000227000	-1.687071000
C	-3.506439000	0.145180000	0.672320000
C	-4.361458000	0.113202000	-1.985587000
C	-4.865572000	0.252186000	0.372193000
C	-5.296664000	0.234140000	-0.956049000
H	-2.280366000	-0.092097000	-2.499574000
H	-3.187687000	0.171425000	1.715013000
H	-4.688858000	0.104839000	-3.026652000
H	-5.589914000	0.354374000	1.182335000
H	-6.359759000	0.317900000	-1.187935000
C	0.308298000	-2.262813000	-1.606185000
Ag	2.247610000	-0.021448000	-0.622133000

Cl	4.313540000	0.706254000	0.122131000
C	-1.091579000	-2.831014000	-1.912843000
H	-1.018521000	-3.899561000	-2.168605000
H	-1.771889000	-2.743997000	-1.052523000
H	-1.560868000	-2.319044000	-2.765771000
C	0.939293000	-3.096350000	-0.476899000
H	0.348231000	-3.063843000	0.447820000
H	1.011408000	-4.150121000	-0.788453000
H	1.952592000	-2.736837000	-0.243361000
C	1.177300000	-2.435828000	-2.867402000
H	2.201867000	-2.075920000	-2.690648000
H	1.227345000	-3.497474000	-3.154249000
H	0.761919000	-1.874155000	-3.718949000

[{(Ph)$_3$PCHCF3}→AgCl]

E= -3634.57142

C	0.246068000	-0.634178000	-1.332864000
P	-0.730892000	0.099874000	-0.043487000
C	-0.371256000	-0.635555000	1.574089000
C	-1.085986000	-1.763658000	2.006835000
C	0.688367000	-0.136190000	2.348903000
C	-0.749608000	-2.377702000	3.213188000
C	1.014508000	-0.755009000	3.555470000
C	0.296126000	-1.871985000	3.988636000
H	-1.892602000	-2.174128000	1.398064000
H	1.272152000	0.718763000	2.003145000
H	-1.301478000	-3.259643000	3.541731000
H	1.844543000	-0.368525000	4.148141000

H	0.559154000	-2.356402000	4.930604000
C	-0.378517000	1.885828000	0.012326000
C	0.348611000	2.531044000	-0.997812000
C	-0.909819000	2.638156000	1.072058000
C	0.541612000	3.912039000	-0.945096000
C	-0.703574000	4.016173000	1.124747000
C	0.020022000	4.655112000	0.114899000
H	0.793591000	1.959597000	-1.812514000
H	-1.475841000	2.149683000	1.866988000
H	1.117601000	4.402860000	-1.730662000
H	-1.107464000	4.590724000	1.959704000
H	0.183394000	5.733132000	0.158762000
H	0.075548000	-0.096066000	-2.276950000
C	-2.548212000	0.024361000	-0.276180000
C	-3.055680000	-0.032500000	-1.582957000
C	-3.440963000	0.124009000	0.803581000
C	-4.432070000	0.005912000	-1.806281000
C	-4.817036000	0.159488000	0.575197000
C	-5.314691000	0.101483000	-0.728539000
H	-2.375714000	-0.123617000	-2.430724000
H	-3.066004000	0.161900000	1.827144000
H	-4.814438000	-0.046511000	-2.826827000
H	-5.502556000	0.230081000	1.421413000
H	-6.391515000	0.126185000	-0.903850000
Ag	2.261451000	-0.174844000	-0.696025000
Cl	4.347606000	0.430127000	0.070273000
C	0.075444000	-2.103647000	-1.592046000
F	0.841215000	-2.494295000	-2.644850000

F	0.409804000	-2.885599000	-0.529317000
F	-1.216861000	-2.475631000	-1.922751000

[{$(Ph)_3PCHCl$}→AgCl]

E= -2141.2741379

C	0.235645000	-0.161552000	-1.560331000
P	-0.749802000	0.041519000	-0.082137000
C	-0.253192000	-1.085560000	1.248286000
C	0.355335000	-2.315724000	0.953143000
C	-0.492012000	-0.725381000	2.584398000
C	0.718331000	-3.173660000	1.990765000
C	-0.124717000	-1.591027000	3.615929000
C	0.479464000	-2.814466000	3.319572000
H	0.555303000	-2.595294000	-0.081545000
H	-0.943448000	0.239965000	2.821184000
H	1.202812000	-4.122752000	1.757416000
H	-0.299491000	-1.300608000	4.653075000
H	0.775730000	-3.485733000	4.127406000
C	-0.503987000	1.746183000	0.494435000
C	0.746291000	2.125264000	1.016183000
C	-1.528245000	2.698935000	0.376498000
C	0.966276000	3.449445000	1.395718000
C	-1.299555000	4.019757000	0.765140000
C	-0.052799000	4.396447000	1.269652000
H	1.551403000	1.393301000	1.115822000
H	-2.504527000	2.409644000	-0.013966000
H	1.942993000	3.736572000	1.787640000
H	-2.099943000	4.755436000	0.671288000

H	0.124202000	5.430983000	1.569199000
H	0.040162000	0.708601000	-2.204080000
C	-2.538810000	-0.201963000	-0.356426000
C	-3.096498000	0.247884000	-1.565058000
C	-3.359538000	-0.832473000	0.590060000
C	-4.460145000	0.088919000	-1.809912000
C	-4.723415000	-0.991248000	0.338388000
C	-5.275297000	-0.528568000	-0.857855000
H	-2.461418000	0.712006000	-2.321704000
H	-2.932689000	-1.209428000	1.520363000
H	-4.884212000	0.437821000	-2.752814000
H	-5.354920000	-1.484225000	1.079304000
H	-6.341038000	-0.658246000	-1.053895000
Ag	2.277332000	-0.104167000	-0.998508000
Cl	4.466276000	0.056513000	-0.296881000
Cl	-0.284921000	-1.633163000	-2.489465000

[{$(Ph)_3$PCHF}→AgCl]

E= -1838.91589

C	0.237666000	0.076273000	-1.661758000
P	-0.766609000	0.028135000	-0.161830000
C	-0.310797000	-1.364066000	0.902460000
C	0.189108000	-2.541702000	0.323300000
C	-0.478940000	-1.280618000	2.293093000
C	0.515250000	-3.625463000	1.137323000
C	-0.146720000	-2.370824000	3.099522000
C	0.348468000	-3.541754000	2.522412000
H	0.336318000	-2.601272000	-0.755839000

H	-0.847407000	-0.359072000	2.747775000
H	0.914957000	-4.535145000	0.687066000
H	-0.264688000	-2.298768000	4.181888000
H	0.616578000	-4.389381000	3.155362000
C	-0.482553000	1.581075000	0.725069000
C	0.759558000	1.807898000	1.345649000
C	-1.467386000	2.581924000	0.743253000
C	1.010377000	3.034158000	1.962374000
C	-1.207694000	3.801819000	1.368575000
C	0.030948000	4.029709000	1.973422000
H	1.532349000	1.035982000	1.339772000
H	-2.436667000	2.407686000	0.274024000
H	1.980621000	3.207527000	2.429825000
H	-1.976243000	4.576244000	1.380442000
H	0.232435000	4.986739000	2.458030000
H	0.023025000	1.037379000	-2.162185000
C	-2.553479000	-0.130749000	-0.505202000
C	-3.067069000	0.469822000	-1.666351000
C	-3.414119000	-0.845526000	0.341877000
C	-4.427039000	0.373409000	-1.962500000
C	-4.773322000	-0.938892000	0.040220000
C	-5.281444000	-0.328062000	-1.108724000
H	-2.400598000	1.003952000	-2.345815000
H	-3.021364000	-1.338840000	1.232131000
H	-4.817046000	0.838960000	-2.869033000
H	-5.436451000	-1.496852000	0.703397000
H	-6.343918000	-0.407885000	-1.344969000
Ag	2.266717000	0.028558000	-1.088030000

Cl	4.454184000	0.031701000	-0.353714000
F	-0.192723000	-0.966776000	-2.530886000

[{(Ph)$_3$PCHH}→AgCl]

E= -2090.25779

C	0.282456000	-0.217730000	-1.537842000
P	-0.691701000	0.066518000	-0.105155000
C	-0.244365000	-1.056666000	1.250939000
C	0.310135000	-2.311751000	0.959533000
C	-0.469610000	-0.687334000	2.585430000
C	0.624714000	-3.191299000	1.994654000
C	-0.147985000	-1.571039000	3.617574000
C	0.395627000	-2.822861000	3.322897000
H	0.527341000	-2.588982000	-0.072921000
H	-0.875602000	0.298433000	2.820651000
H	1.068101000	-4.160573000	1.762304000
H	-0.311403000	-1.273595000	4.654655000
H	0.655738000	-3.508416000	4.131147000
C	-0.490808000	1.774986000	0.488796000
C	0.789359000	2.234779000	0.844713000
C	-1.590794000	2.640983000	0.586082000
C	0.960913000	3.549452000	1.276666000
C	-1.409826000	3.955947000	1.020515000
C	-0.135733000	4.411461000	1.363389000
H	1.654620000	1.569006000	0.771642000
H	-2.589493000	2.292609000	0.320256000
H	1.959832000	3.897863000	1.543425000
H	-2.269710000	4.624405000	1.088350000

H	0.004017000	5.440062000	1.700863000
H	0.091005000	0.589198000	-2.260272000
C	-2.489831000	-0.176091000	-0.379031000
C	-3.024612000	0.191803000	-1.624825000
C	-3.337056000	-0.727489000	0.594089000
C	-4.384852000	0.024861000	-1.885986000
C	-4.696698000	-0.899266000	0.326277000
C	-5.223117000	-0.520977000	-0.910525000
H	-2.371572000	0.602585000	-2.397356000
H	-2.933832000	-1.035816000	1.559693000
H	-4.788673000	0.314786000	-2.857491000
H	-5.345570000	-1.335619000	1.087661000
H	-6.285663000	-0.658904000	-1.117933000
Ag	2.347462000	-0.192598000	-1.032175000
Cl	4.583481000	-0.132042000	-0.462225000
H	0.013659000	-1.185482000	-1.986743000

[{(Ph)$_3$PCHMe}→AgCl]

E= -1721.1128376

C	0.242754000	-0.073570000	-1.734463000
P	-0.720194000	-0.002173000	-0.258153000
C	-0.336577000	-1.405247000	0.832623000
C	-0.980067000	-2.640920000	0.659645000
C	0.701332000	-1.286572000	1.771056000
C	-0.592759000	-3.742667000	1.425296000
C	1.077654000	-2.389274000	2.536953000
C	0.432242000	-3.616561000	2.365076000
H	-1.780128000	-2.747976000	-0.074572000

H	1.230237000	-0.339109000	1.887142000
H	-1.090891000	-4.702750000	1.280618000
H	1.891223000	-2.290258000	3.256707000
H	0.735096000	-4.479761000	2.960375000
C	-0.448484000	1.552532000	0.650685000
C	0.368732000	2.565553000	0.129825000
C	-1.104965000	1.752775000	1.875461000
C	0.526378000	3.763419000	0.828360000
C	-0.934381000	2.947091000	2.574723000
C	-0.119970000	3.954442000	2.050956000
H	0.909176000	2.407120000	-0.804499000
H	-1.747293000	0.974247000	2.290886000
H	1.171149000	4.542444000	0.419140000
H	-1.438693000	3.089963000	3.531787000
H	0.014584000	4.887879000	2.600205000
H	0.081185000	0.863442000	-2.292687000
C	-2.539807000	-0.051098000	-0.526782000
C	-3.027382000	0.468209000	-1.735941000
C	-3.451557000	-0.526708000	0.429754000
C	-4.399951000	0.515852000	-1.983689000
C	-4.823702000	-0.477893000	0.179409000
C	-5.299864000	0.042774000	-1.026432000
H	-2.326389000	0.838691000	-2.486922000
H	-3.091673000	-0.945701000	1.370912000
H	-4.766212000	0.920309000	-2.928796000
H	-5.523653000	-0.850256000	0.929593000
H	-6.373218000	0.076760000	-1.220859000
C	-0.026492000	-1.310388000	-2.602892000

H	0.642895000	-1.297533000	-3.473484000
H	0.182866000	-2.240975000	-2.056101000
H	-1.063099000	-1.370718000	-2.981823000
Ag	2.261053000	0.012901000	-0.999657000
Cl	4.429262000	0.108229000	-0.208777000

[{$(Ph)_3$PCHPh}→AgCl]

E= -1912.6787894

C	0.240919000	-0.522111000	-1.373685000
P	-0.721002000	-0.125825000	0.059608000
C	-0.329013000	-1.075261000	1.563507000
C	0.370292000	-2.289249000	1.495539000
C	-0.719597000	-0.568476000	2.814492000
C	0.661197000	-2.993435000	2.664231000
C	-0.422107000	-1.275996000	3.979856000
C	0.265253000	-2.489723000	3.905016000
H	0.716109000	-2.671156000	0.533513000
H	-1.233195000	0.392753000	2.881112000
H	1.217880000	-3.929436000	2.602609000
H	-0.715084000	-0.869120000	4.949063000
H	0.507138000	-3.036419000	4.818042000
C	-0.418173000	1.623260000	0.461907000
C	0.835803000	2.001905000	0.973206000
C	-1.400419000	2.598757000	0.233962000
C	1.103259000	3.346824000	1.230241000
C	-1.125465000	3.941436000	0.500674000
C	0.125821000	4.316591000	0.993955000
H	1.607294000	1.250444000	1.160915000

H	-2.380807000	2.312626000	-0.148881000
H	2.082671000	3.632428000	1.616800000
H	-1.893994000	4.694949000	0.320686000
H	0.338946000	5.367278000	1.198921000
H	0.326080000	0.422117000	-1.934888000
C	-2.522919000	-0.312830000	-0.220028000
C	-3.019939000	0.021594000	-1.491454000
C	-3.407529000	-0.787290000	0.759654000
C	-4.382181000	-0.094288000	-1.767233000
C	-4.769693000	-0.905793000	0.477090000
C	-5.259331000	-0.556033000	-0.782853000
H	-2.335643000	0.356861000	-2.272988000
H	-3.034234000	-1.077164000	1.742368000
H	-4.756293000	0.164071000	-2.759171000
H	-5.449209000	-1.278537000	1.245436000
H	-6.323926000	-0.654267000	-1.002180000
Ag	2.279401000	-0.644808000	-0.660684000
Cl	4.446556000	-0.699071000	0.133565000
C	-0.136462000	-1.657866000	-2.261022000
C	0.229567000	-1.596672000	-3.622687000
C	-0.836576000	-2.802294000	-1.833298000
C	-0.078064000	-2.628960000	-4.504724000
C	-1.143264000	-3.838138000	-2.718017000
C	-0.766281000	-3.761899000	-4.059169000
H	0.782500000	-0.725550000	-3.982961000
H	-1.161612000	-2.891623000	-0.794180000
H	0.226532000	-2.549479000	-5.550296000
H	-1.686028000	-4.711680000	-2.350959000

H	-1.004033000	-4.573125000	-4.748796000

[{(Ph)$_3$PCHSi(CH3)3}→AgCl]

E= -1681.85031

C	0.306554000	-0.735704000	-1.076572000
P	-0.789640000	0.173785000	-0.070327000
C	-0.619332000	-0.284146000	1.681722000
C	-1.560220000	-1.121717000	2.299533000
C	0.512906000	0.137880000	2.399452000
C	-1.368267000	-1.536251000	3.619104000
C	0.695745000	-0.277364000	3.718331000
C	-0.241901000	-1.114924000	4.328538000
H	-2.441790000	-1.455975000	1.750910000
H	1.262044000	0.776118000	1.923563000
H	-2.101322000	-2.192767000	4.090718000
H	1.581234000	0.050171000	4.264996000
H	-0.092540000	-1.441476000	5.359246000
C	-0.542693000	1.980413000	-0.194082000
C	-0.098689000	2.529890000	-1.406260000
C	-0.845897000	2.830583000	0.879461000
C	0.035258000	3.910693000	-1.542201000
C	-0.700533000	4.212507000	0.741040000
C	-0.263969000	4.753900000	-0.468969000
H	0.168147000	1.877176000	-2.239020000
H	-1.169633000	2.416303000	1.835722000
H	0.391466000	4.327676000	-2.485347000
H	-0.920248000	4.865770000	1.587160000

H	-0.144313000	5.833565000	-0.572955000
H	0.128266000	-0.468532000	-2.132429000
C	-2.569959000	-0.015409000	-0.492007000
C	-2.931403000	-0.766251000	-1.617297000
C	-3.570826000	0.639107000	0.246300000
C	-4.272055000	-0.871372000	-1.996707000
C	-4.908354000	0.527359000	-0.129772000
C	-5.261328000	-0.227769000	-1.252894000
H	-2.158637000	-1.272232000	-2.196632000
H	-3.306789000	1.241957000	1.116878000
H	-4.541067000	-1.459848000	-2.875567000
H	-5.678597000	1.036517000	0.452176000
H	-6.308838000	-0.310152000	-1.547974000
Ag	2.237908000	0.108450000	-0.591732000
Cl	4.287091000	1.001827000	-0.011705000
Si	0.600975000	-2.604982000	-0.924615000
C	1.724627000	-3.055571000	-2.372405000
H	2.695785000	-2.545080000	-2.297525000
H	1.910235000	-4.140654000	-2.388685000
H	1.271751000	-2.780618000	-3.337272000
C	1.432380000	-3.083419000	0.698662000
H	0.798537000	-2.878953000	1.573128000
H	1.646266000	-4.164057000	0.687755000
H	2.383919000	-2.549477000	0.835898000
C	-0.972021000	-3.657238000	-1.075800000
H	-0.711754000	-4.721230000	-0.958303000
H	-1.715876000	-3.413272000	-0.302600000
H	-1.457688000	-3.547379000	-2.057010000

[{(Ph)$_3$PCHSiH3}→AgCl]

E= -1912.67879

C	0.254236000	-0.497482000	-1.525917000
P	-0.737850000	0.025707000	-0.184839000
C	-0.623202000	-1.147039000	1.199891000
C	-1.707020000	-1.975682000	1.526166000
C	0.583006000	-1.262187000	1.912668000
C	-1.582742000	-2.915968000	2.551021000
C	0.698125000	-2.203564000	2.934730000
C	-0.382205000	-3.030872000	3.253984000
H	-2.646844000	-1.890090000	0.979162000
H	1.437618000	-0.628351000	1.660480000
H	-2.427746000	-3.561084000	2.796844000
H	1.640167000	-2.291484000	3.477909000
H	-0.286519000	-3.767966000	4.053317000
C	-0.268845000	1.672310000	0.441506000
C	0.229907000	2.629099000	-0.455555000
C	-0.438384000	2.010199000	1.792329000
C	0.548676000	3.909231000	-0.006347000
C	-0.110791000	3.292838000	2.237777000
C	0.379025000	4.242667000	1.340197000
H	0.395004000	2.367807000	-1.502129000
H	-0.802653000	1.266001000	2.502872000
H	0.947094000	4.643608000	-0.707865000
H	-0.228596000	3.544353000	3.293073000
H	0.642838000	5.241326000	1.692101000
H	0.075575000	0.147326000	-2.400964000

C	-2.518273000	0.189416000	-0.594953000
C	-3.022543000	-0.451502000	-1.736268000
C	-3.386570000	0.949261000	0.206725000
C	-4.375586000	-0.341338000	-2.065698000
C	-4.736940000	1.054545000	-0.124969000
C	-5.234035000	0.408964000	-1.260796000
H	-2.356710000	-1.041708000	-2.367121000
H	-3.006722000	1.472547000	1.085629000
H	-4.756422000	-0.843853000	-2.956373000
H	-5.402369000	1.650128000	0.502382000
H	-6.290434000	0.496839000	-1.520516000
Ag	2.286151000	-0.180103000	-0.879315000
Cl	4.428212000	0.171409000	-0.105708000
Si	0.323174000	-2.310436000	-1.999545000
H	1.292856000	-2.462544000	-3.125663000
H	0.742442000	-3.155500000	-0.842278000
H	-0.988995000	-2.873364000	-2.488764000