

## SUPPLEMENTARY MATERIAL

# Antimicrobial activity of anionic bis(N-heterocyclic carbene)silver complexes

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**Figure S1.** IR spectra of compounds **1f,g** and complexes **2f,g**.

**Figure S2.** <sup>1</sup>H NMR and <sup>13</sup>C{<sup>1</sup>H} NMR spectra of compounds **1f-g**.

**Figure S3.** Optimized structures of compounds **1f-g** and ligands NHC<sup>β-Me</sup> and NHC<sup>GlyGly</sup>.

**Figure S4.** Optimized structures of complexes: (a) [Ag(NHC<sup>β-Me</sup>)<sub>2</sub>]<sup>3-</sup>; (b) [Ag(NHC<sup>GlyGly</sup>)<sub>2</sub>]<sup>3-</sup>; and (c) Na<sub>3</sub>[Ag(NHC<sup>β-Me</sup>)<sub>2</sub>], **2g**. Two views of each complex are shown.

**Figure S5.** Comparison of the calculated and experimental <sup>1</sup>H and <sup>13</sup>C NMR spectra for **2f**.

**Figure S6.** Comparison of the calculated and experimental <sup>1</sup>H and <sup>13</sup>C NMR spectra for **2g**.

**Table S1.** Comparison of experimental selected structural parameters of complexes **2c** and **2g** with the calculated parameters for the anions [Ag(NHC<sup>R</sup>)<sub>2</sub>]<sup>3-</sup> of these complexes.

**Table S2.** (a) Selected structural data of complex **1f**. (b) Selected structural data of complex **2c**. (c) Selected structural data of complex **2g**. Bond distances (Å) and angles (°).

**Table S3.** Specific rotations [ $\alpha$ ]<sub>D</sub> for complexes **2**.

**Figure S7.** Crystal packing views of complex **1f**.

**Figure S8.** Crystal packing views of complex **2c**.

**Figure S9.** Crystal packing views of complex **2g** viewed along *b* axis.

**Table S4.** Optimized structures of complexes  $[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{R}})]^{2-}$  and their calculated properties.

**Figure S10.** Correlation between calculated TEP values ( $v_{\text{CO}}$ ) of the  $\text{NHC}^{\text{R}}$  carbenes and the MO energy of the  $\sigma$  lone pair orbitals.

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**Figure S15.** Qualitative hemolysis test of complex **2a** and several control chemicals ( $\text{AgNO}_3$ ,  $\text{H}_2\text{O}_2$ , sodium dodecyl sulfate, SDS and NaOH) for comparison.

**Table S8.** Crystal data and structure refinement for **1f**.

**Table S9.** Crystal data and structure refinement for **2c**.

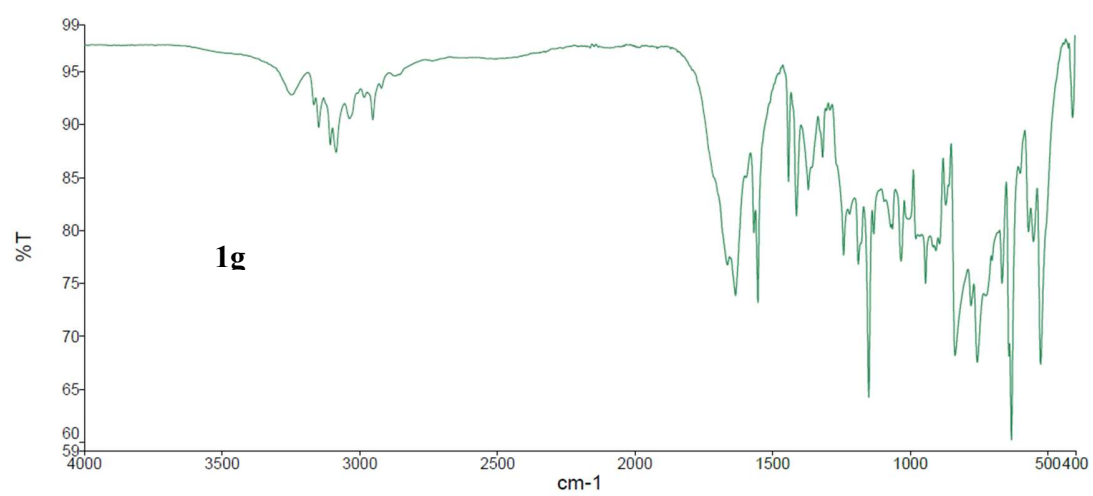
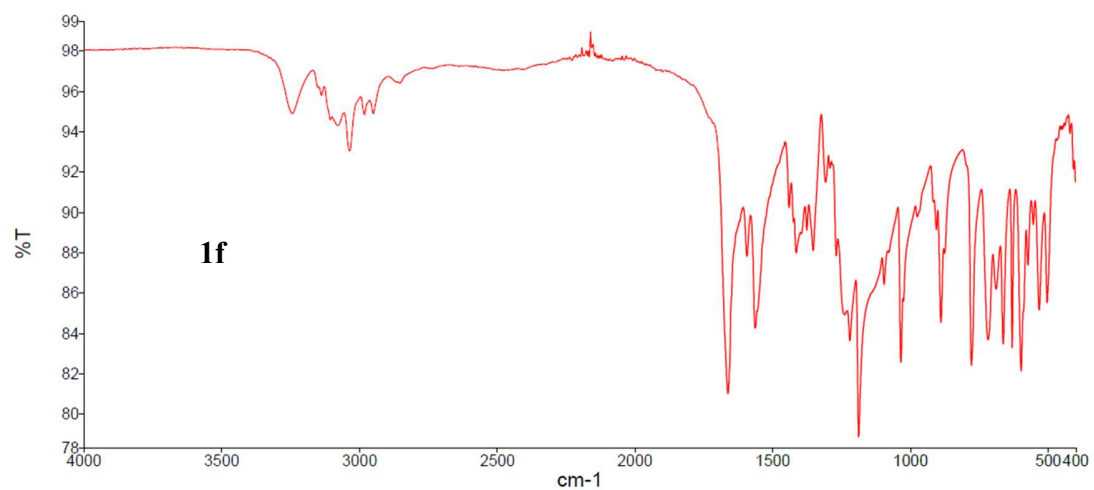
**Table S10.** Crystal data and structure refinement for **2g**.

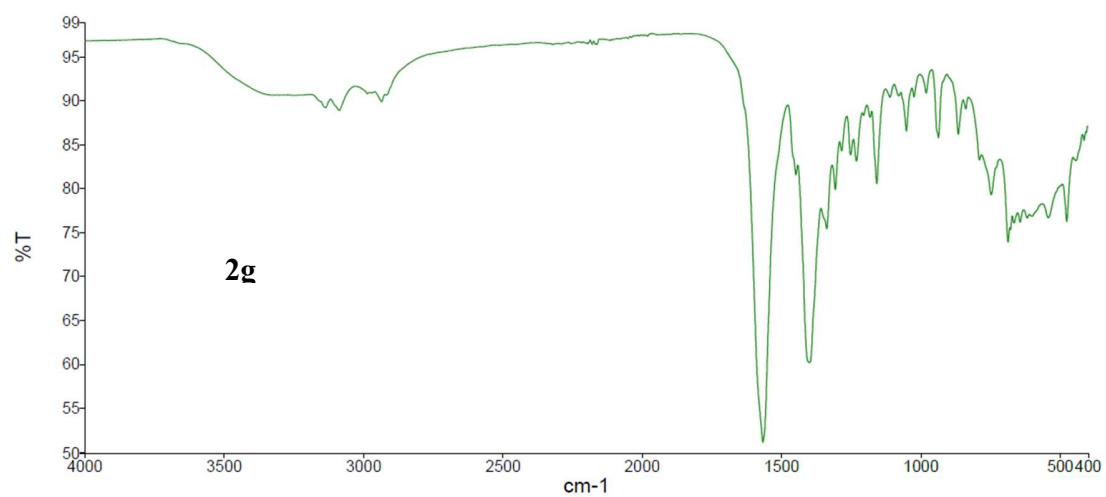
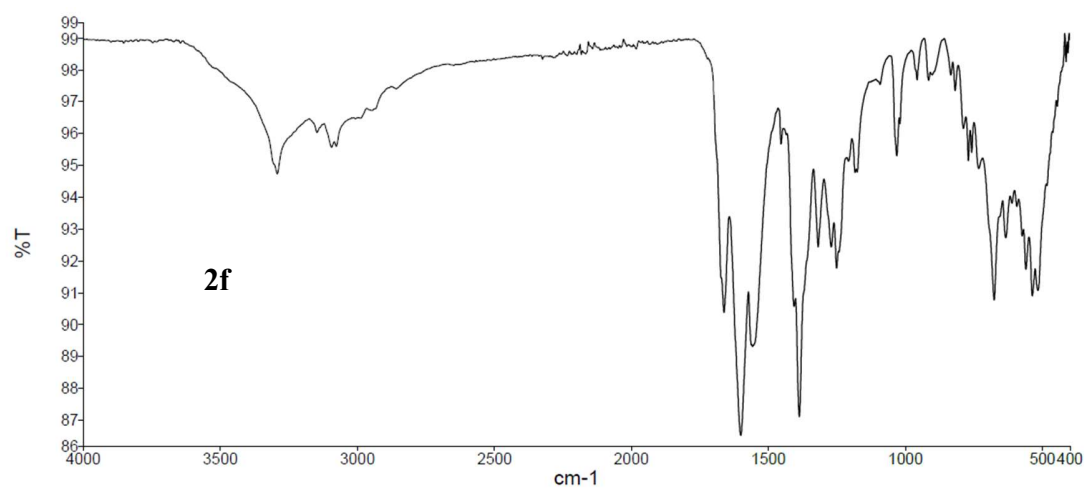
**Table S11.** Coordinates and optimized structures of NHC-silver complexes used for the correlation between calculated and experimental  $^{109}\text{Ag}$  NMR chemical shifts.

**Table S12.** Coordinates of complexes  $[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{R}})]^{2-}$  used for the determination of the Tolman Electronic Parameter (TEP).

**Table S13.** Coordinates of the optimized structures.

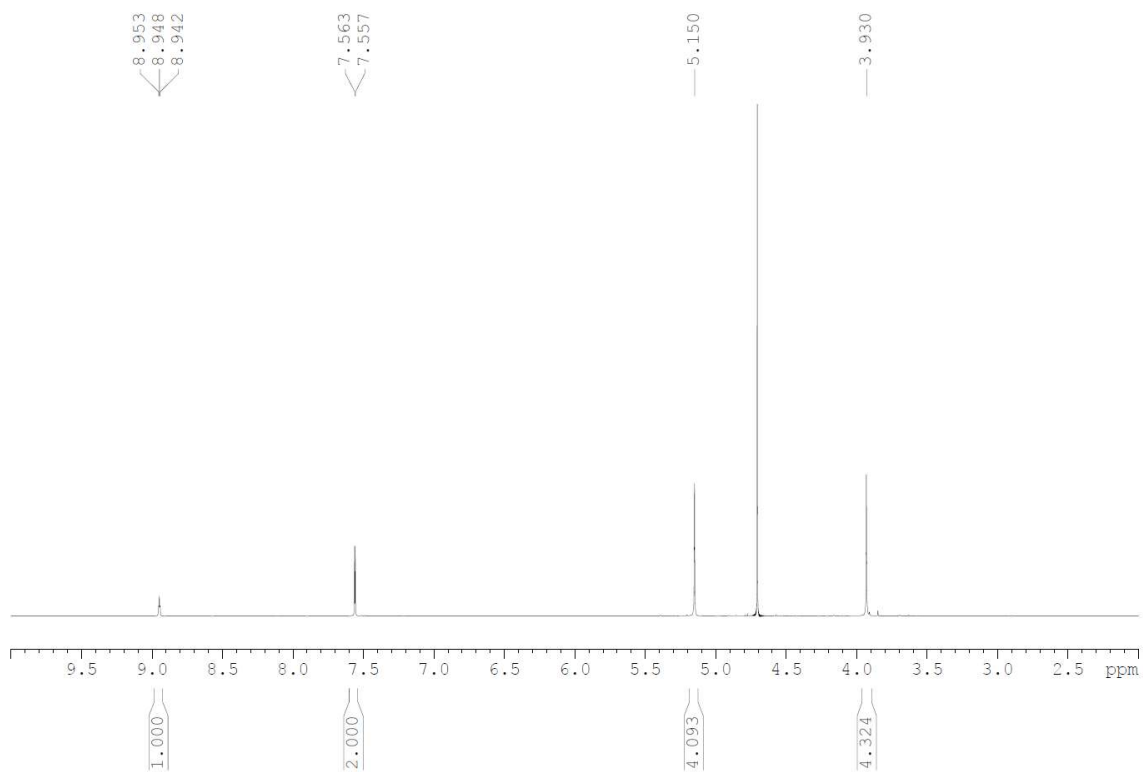
**Figure S1.** IR spectra of compounds **1f,g** and complexes **2f,g**.



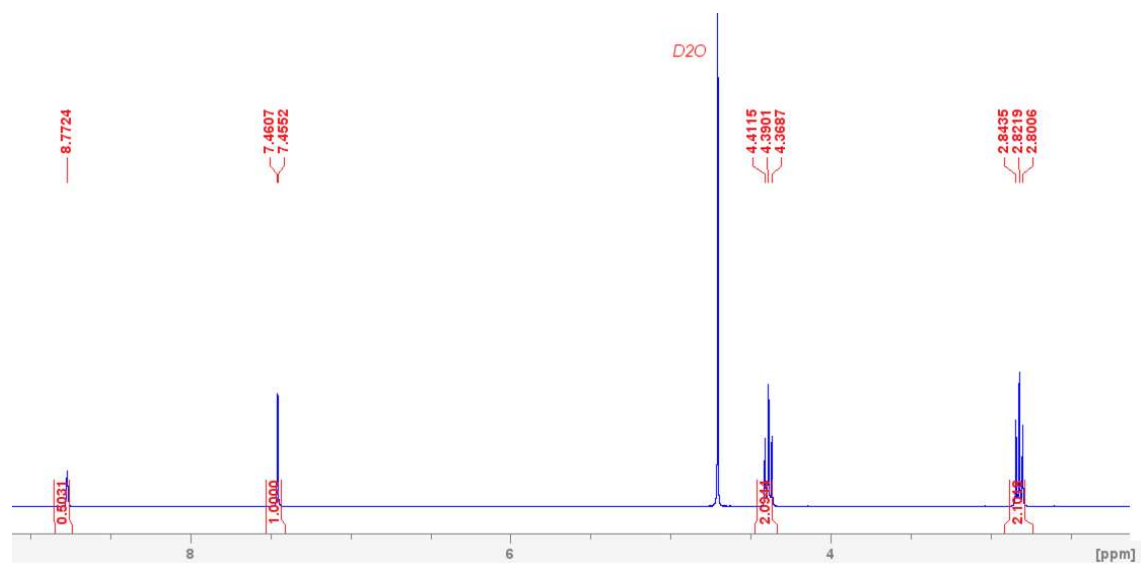


**Figure S2.**  $^1\text{H}$  NMR spectra of compounds **1f-g**.

**1f**

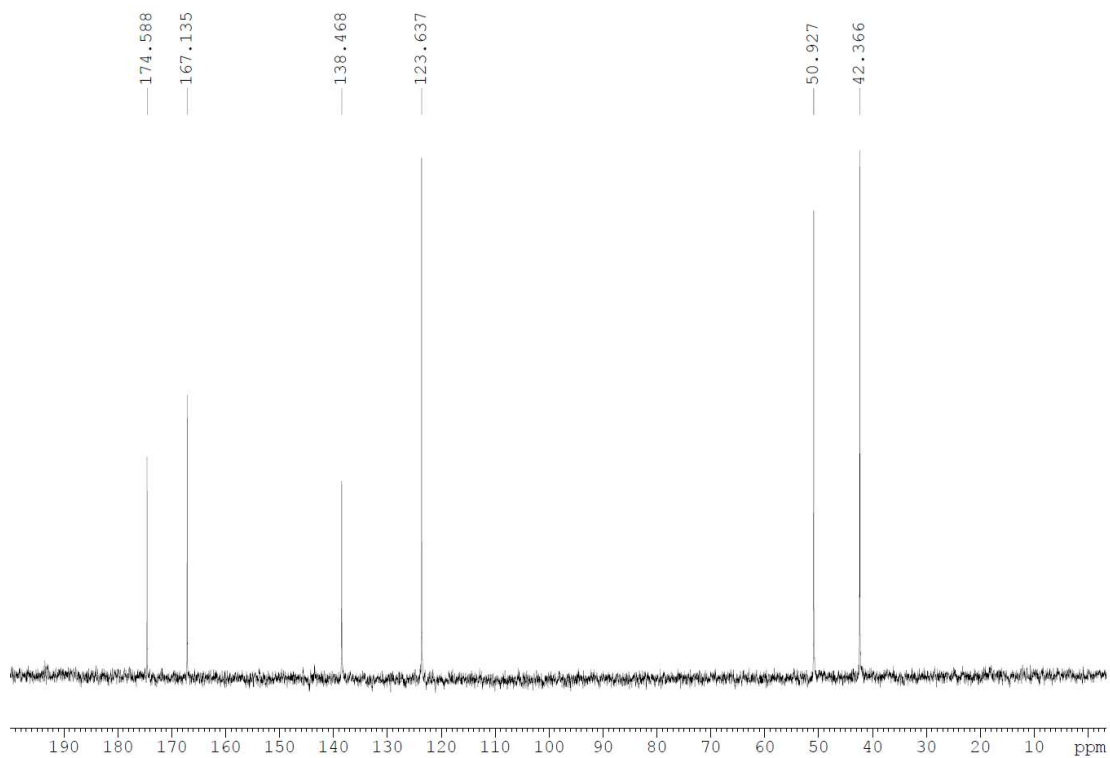


**1g**

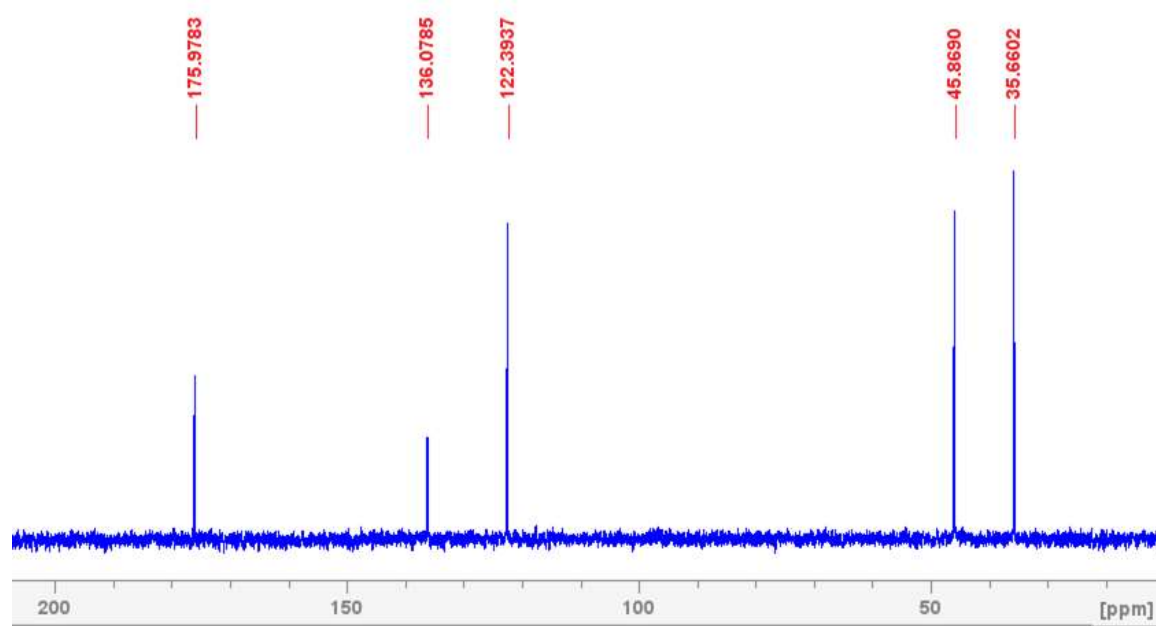


**Figure S2.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectra of compounds **1f-g**.

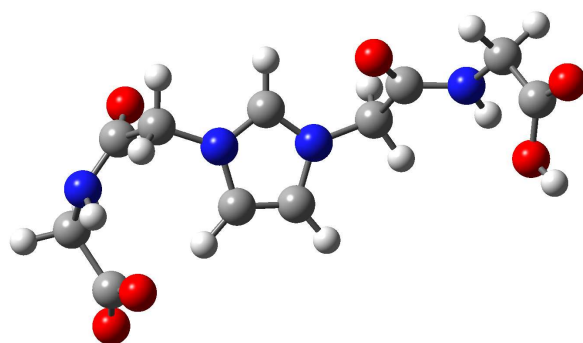
**1f**



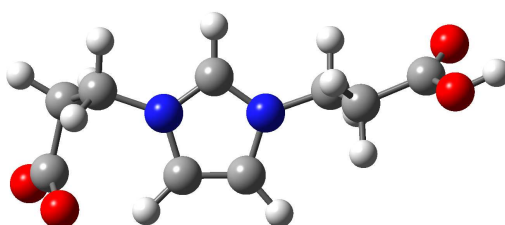
**1g**



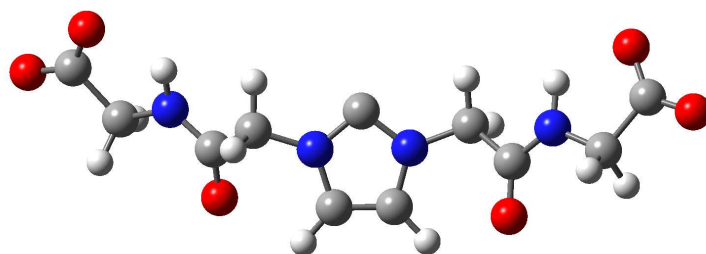
**Figure S3.** Optimized structures of compounds **1f-g** and ligands  $\text{NHC}^{\text{GlyGly}}$  and  $\text{NHC}^{\beta\text{-Me}}$ .



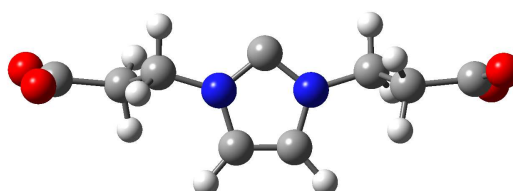
**1f**



**1g**

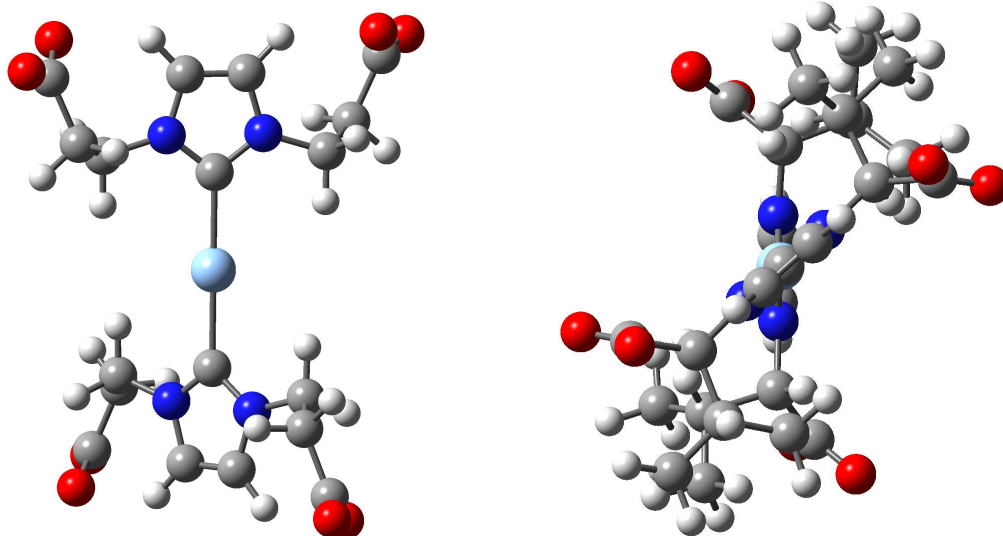


$\text{NHC}^{\text{GlyGly}}$

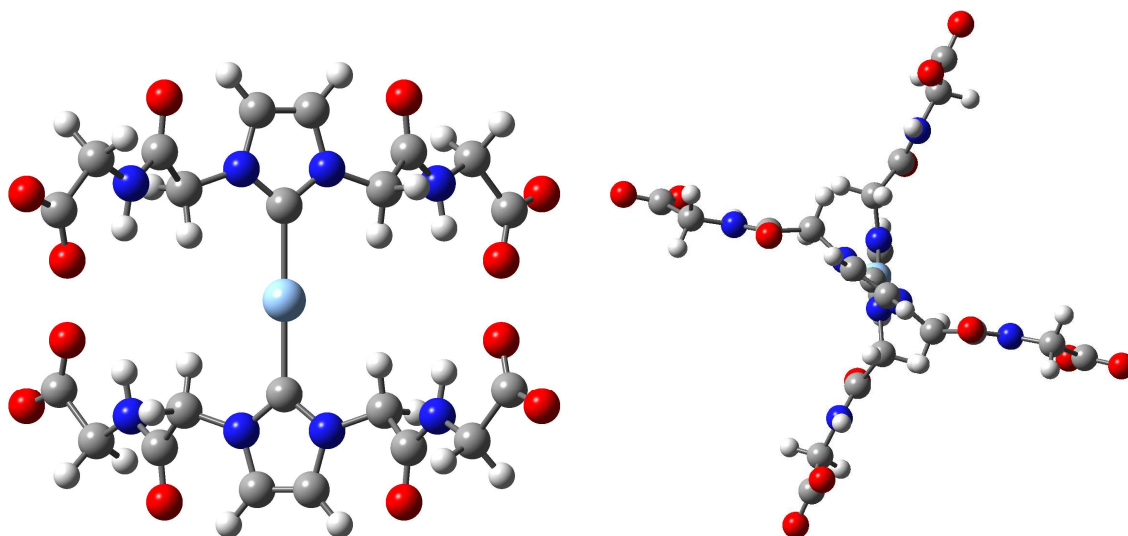


$\text{NHC}^{\beta\text{-Me}}$

**Figure S4.** Optimized structures of complexes: (a)  $[\text{Ag}(\text{NHC}^{\beta\text{-Me}})_2]^{3-}$ ; (b)  $[\text{Ag}(\text{NHC}^{\text{GlyGly}})_2]^{3-}$ ; and (c)  $\text{Na}_3[\text{Ag}(\text{NHC}^{\beta\text{-Me}})_2]$ , **2g**. Two views of each complex are shown.

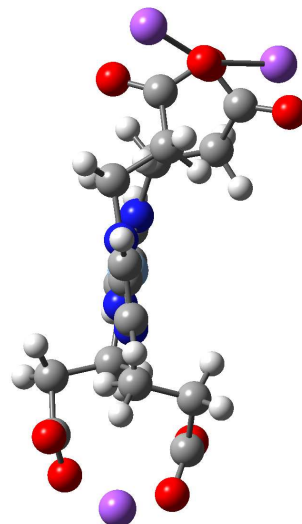
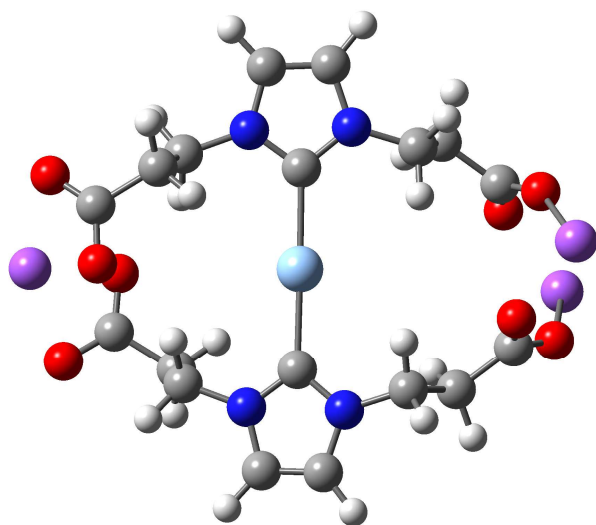


(a)



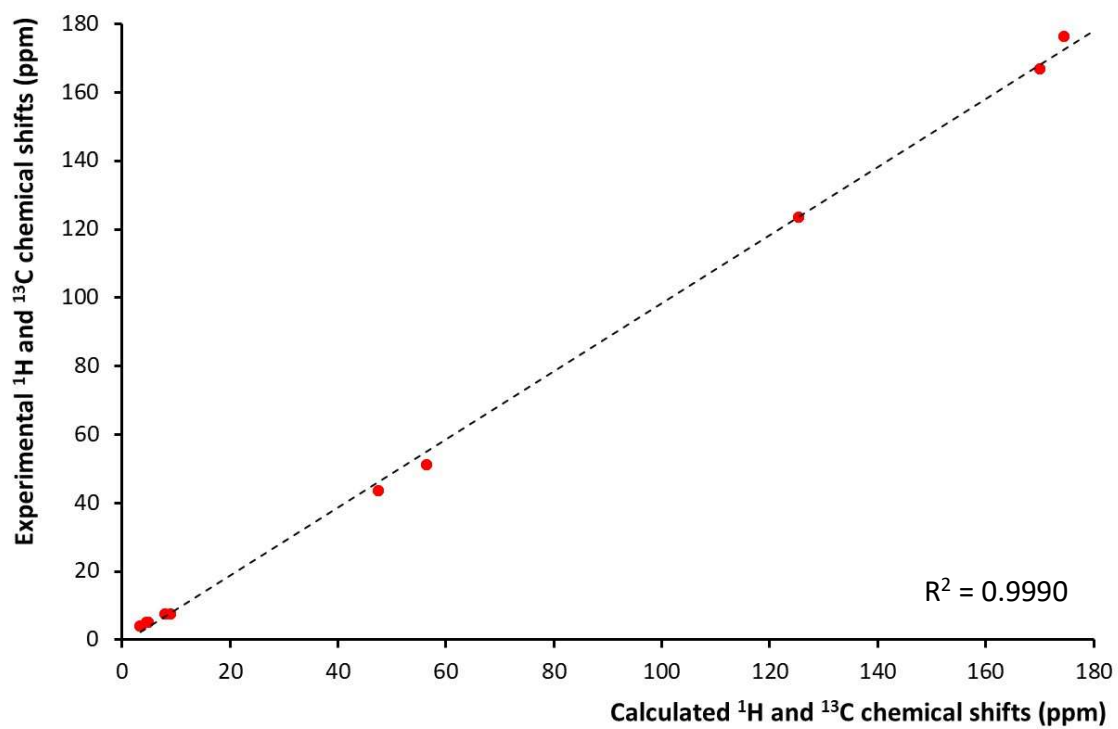
(b)



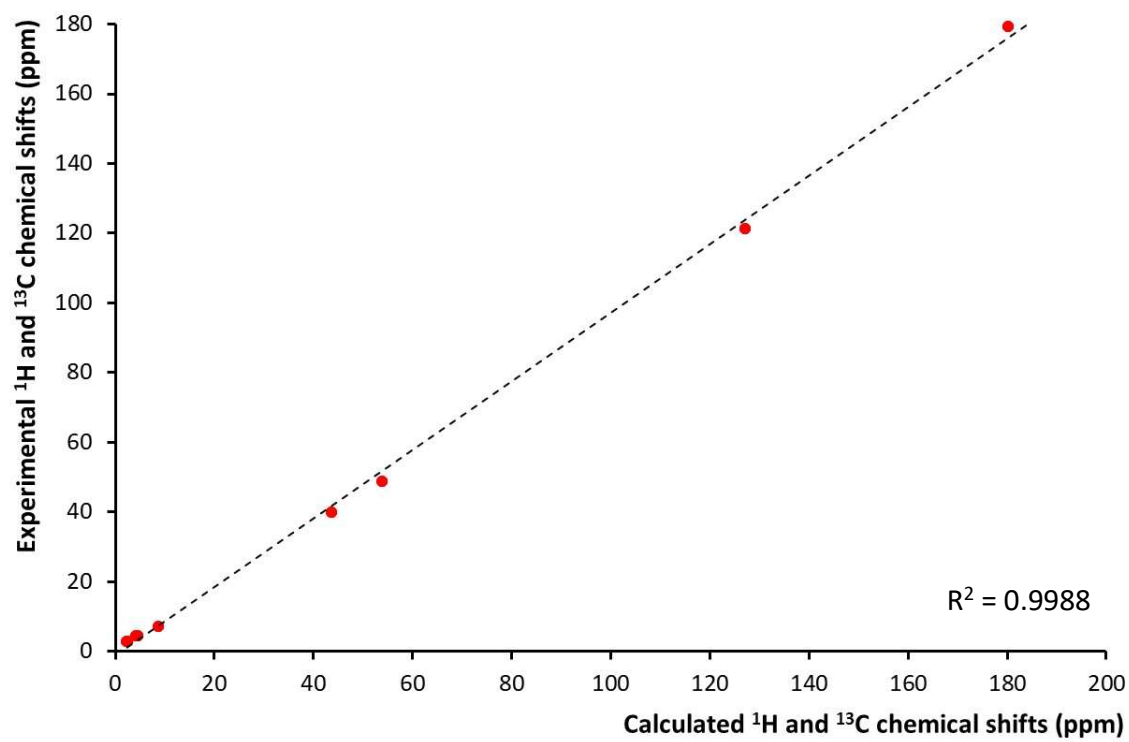


(c)

**Figure S5.** Comparison of the calculated and experimental  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for **2f**.



**Figure S6.** Comparison of the calculated and experimental  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra for **2g**.



**Table S1.** Comparison of experimental selected structural parameters of complexes **2c** and **2g** with the calculated parameters for the anions  $[\text{Ag}(\text{NHC}^{\text{R}})_2]^{3-}$  of these complexes.

Bond distances (Å) and angles (°)	2c		2g	
	Exp.	Calc.	Exp.	Calc.
Ag-C <sub>carbene</sub>	2.12(1) 2.15(1)	2.171	2.081(2) 2.084(2)	2.151
C-O <sub>carboxylate</sub>	1.24(2) 1.34(2) 1.28(1) 1.26(2) 1.28(1) 1.29(2) 1.21(2) 1.29(2)	1.248 1.258	1.245(3) 1.253(3) 1.253(3) 1.232(3) 1.249(3) 1.263(3) 1.252(3) 1.244(3)	1.246 1.259
C <sub>carbene</sub> ≡N	1.41(2) 1.34(2) 1.39(1) 1.41(2)	1.365	1.350(3) 1.352(3)	1.359
C≡C (NHC ring)	1.37(2) 1.39(2)	1.355	1.348(4) 1.352(4)	1.358
C <sub>carbene</sub> -Ag-C <sub>carbene</sub>	174.5(4)	179.1	175.39(9)	179.9

**Table S2. (a)** Selected structural data of complex **1f** [bond distances (Å) and angles (°)].

O(1)-C(5)	1.235(8)	O(10)-C(20)	1.241(8)
O(2)-C(7)	1.231(8)	O(11)-C(22)	1.239(8)
O(3)-C(7)	1.265(8)	O(12)-C(22)	1.234(8)
O(4)-C(9)	1.251(9)		
O(5)-C(11)	1.199(9)	O(2)-C(7)-O(3)	124.5(6)
O(6)-C(11)	1.279(9)	O(5)-C(11)-O(6)	125.3(7)
O(7)-C(16)	1.241(9)	O(8)-C(18)-O(9)	125.6(7)
O(8)-C(18)	1.202(9)	O(12)-C(22)-O(11)	127.6(7)
O(9)-C(18)	1.301(9)		

**Table S2. (b)** Selected structural data of complex **2c** [bond distances (Å) and angles (°)].

Ag(1A)-C(14A)	2.123(11)	O(3C)-C(10C)	1.268(15)
Ag(1A)-C(1A)	2.148(12)	O(4C)-C(10C)	1.294(15)
O(1A)-C(5A)	1.241(17)	O(5C)-C(18C)	1.270(15)
O(2A)-C(5A)	1.336(17)	O(6C)-C(18C)	1.297(16)
O(3A)-C(10A)	1.278(14)	O(7C)-C(23C)	1.22(3)
O(4A)-C(10A)	1.258(15)	O(8C)-C(23C)	1.26(2)
O(5A)-C(18A)	1.280(14)	Ag(1D)-C(1D)	2.149(11)
O(6A)-C(18A)	1.287(15)	Ag(1D)-C(14D)	2.178(10)
O(7A)-C(23A)	1.21(2)	O(1D)-C(5D)	1.250(18)
O(8A)-C(23A)	1.29(2)	O(2D)-C(5D)	1.15(2)
Ag(1B)-C(14B)	2.163(11)	O(3D)-C(10D)	1.20(2)
Ag(1B)-C(1B)	2.172(12)	O(4D)-C(10D)	1.24(2)
O(1B)-C(5B)	1.189(17)	O(5D)-C(18D)	1.25(2)
O(1B)-Na(6)	2.341(15)	O(6D)-C(18D)	1.34(2)
O(2B)-C(5B)	1.306(18)	O(6D)-Na(10)	2.911(19)
O(3B)-C(10B)	1.297(15)	O(7D)-C(23D)	1.270(15)
O(3B)-Na(3)	2.603(10)	O(8D)-C(23D)	1.267(14)
O(4B)-C(10B)	1.249(15)		
C(20B)-C(19B)	1.538(18)	C(14A)-Ag(1A)-C(1A)	174.5(4)
Ag(1C)-C(1C)	2.130(11)	C(14B)-Ag(1B)-C(1B)	175.3(4)
Ag(1C)-C(14C)	2.132(12)	C(1C)-Ag(1C)-C(14C)	178.4(4)
O(1C)-C(5C)	1.303(17)	C(1D)-Ag(1D)-C(14D)	175.6(4)
O(2C)-C(5C)	1.247(17)		

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

**Table S2. (c)** Selected structural data of complex **2g** [bond distances (Å) and angles (°)].

Ag(1)-C(1)	2.081(2)	N(1)-C(1)	1.350(3)
Ag(1)-C(10)	2.084(2)	N(1)-C(2)	1.382(3)
O(1)-C(6)	1.245(3)	N(1)-C(4)	1.472(3)
O(2)-C(6)	1.253(3)	N(2)-C(1)	1.350(3)
O(3)-C(9)	1.253(3)	N(2)-C(3)	1.381(3)
O(4)-C(9)	1.232(3)	N(2)-C(7)	1.463(3)
O(5)-C(15)	1.249(3)	N(3)-C(10)	1.350(3)
O(6)-C(15)	1.263(3)	N(3)-C(11)	1.380(3)
O(7)-C(18)	1.252(3)	N(3)-C(13)	1.467(3)
O(8)-C(18)	1.244(3)	N(4)-C(10)	1.352(3)
Na(1)-O(9)	2.303(2)	N(4)-C(12)	1.378(3)
Na(1)-O(5)	2.3284(19)	N(4)-C(16)	1.461(3)
Na(1)-O(7)#1	2.341(2)	C(2)-C(3)	1.348(4)
Na(1)-O(10)	2.388(2)	C(4)-C(5)	1.511(3)
Na(1)-O(2)#2	2.5723(19)	C(5)-C(6)	1.516(3)
Na(1)-O(14)#3	2.724(2)	C(7)-C(8)	1.521(3)
Na(2)-O(11)	2.359(2)	C(8)-C(9)	1.530(3)
Na(2)-O(12)	2.3638(19)	C(11)-C(12)	1.352(4)
Na(2)-O(11)#4	2.3880(19)	C(13)-C(14)	1.500(3)
Na(2)-O(10)	2.3963(19)	C(14)-C(15)	1.515(3)
Na(2)-O(2)#2	2.450(2)	C(16)-C(17)	1.519(4)
Na(2)-O(5)	2.492(2)	C(17)-C(18)	1.526(3)
Na(3)-O(14)	2.342(2)	C(1)-Ag(1)-C(10)	175.39(9)
Na(3)-O(12)	2.358(2)	O(1)-C(6)-O(2)	123.5(2)
Na(3)-O(13)	2.383(2)	O(4)-C(9)-O(3)	125.1(2)
Na(3)-O(9)#5	2.465(2)	O(5)-C(15)-O(6)	124.5(2)
Na(3)-O(6)	2.489(2)	O(8)-C(18)-O(7)	125.5(2)
Na(3)-O(1)#6	2.757(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+1,-z; #3 x-1,y,z;  
#4 -x+1,-y+2,-z; #5 x+1,y,z; #6 -x+2,-y+1,-z.

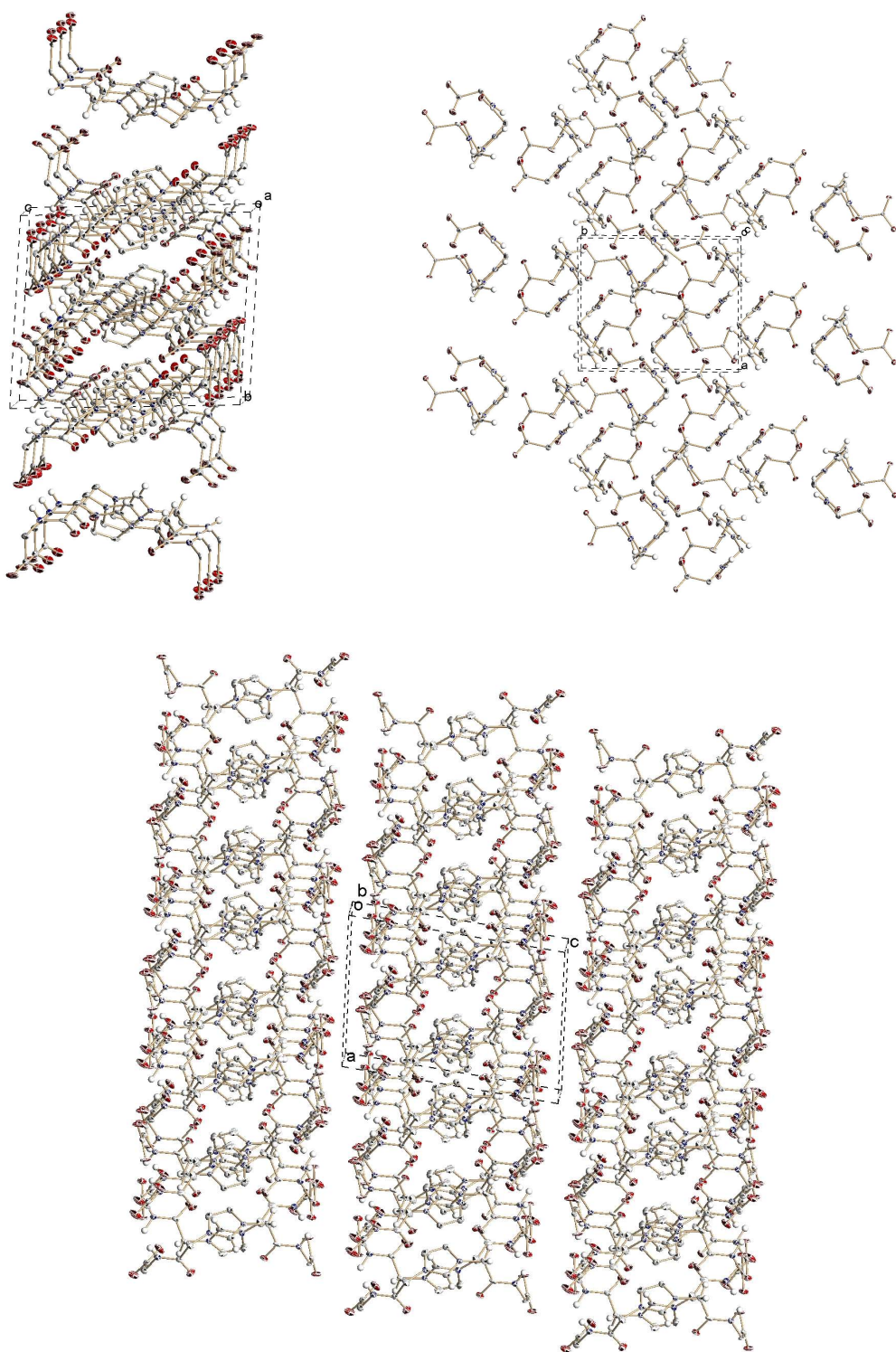
**Table S3.** Specific rotations  $[\alpha]_{\text{D}}$  for complexes **2**.

Complex $\text{Na}_3[\text{Ag}(\text{NHC}^{\text{R}})_2]$	$[\alpha]_{\text{D}}$
<b>2b</b>	$6.5^\circ \pm 0.6$
<b>2b'</b>	$-1.4^\circ \pm 0.3$
<b>2c</b>	$4.1^\circ \pm 0.2$
<b>2c'</b>	$-1.5^\circ \pm 0.2$
<b>2d</b>	$6.8^\circ \pm 0.2$
<b>2e</b>	$18.4^\circ \pm 0.3$

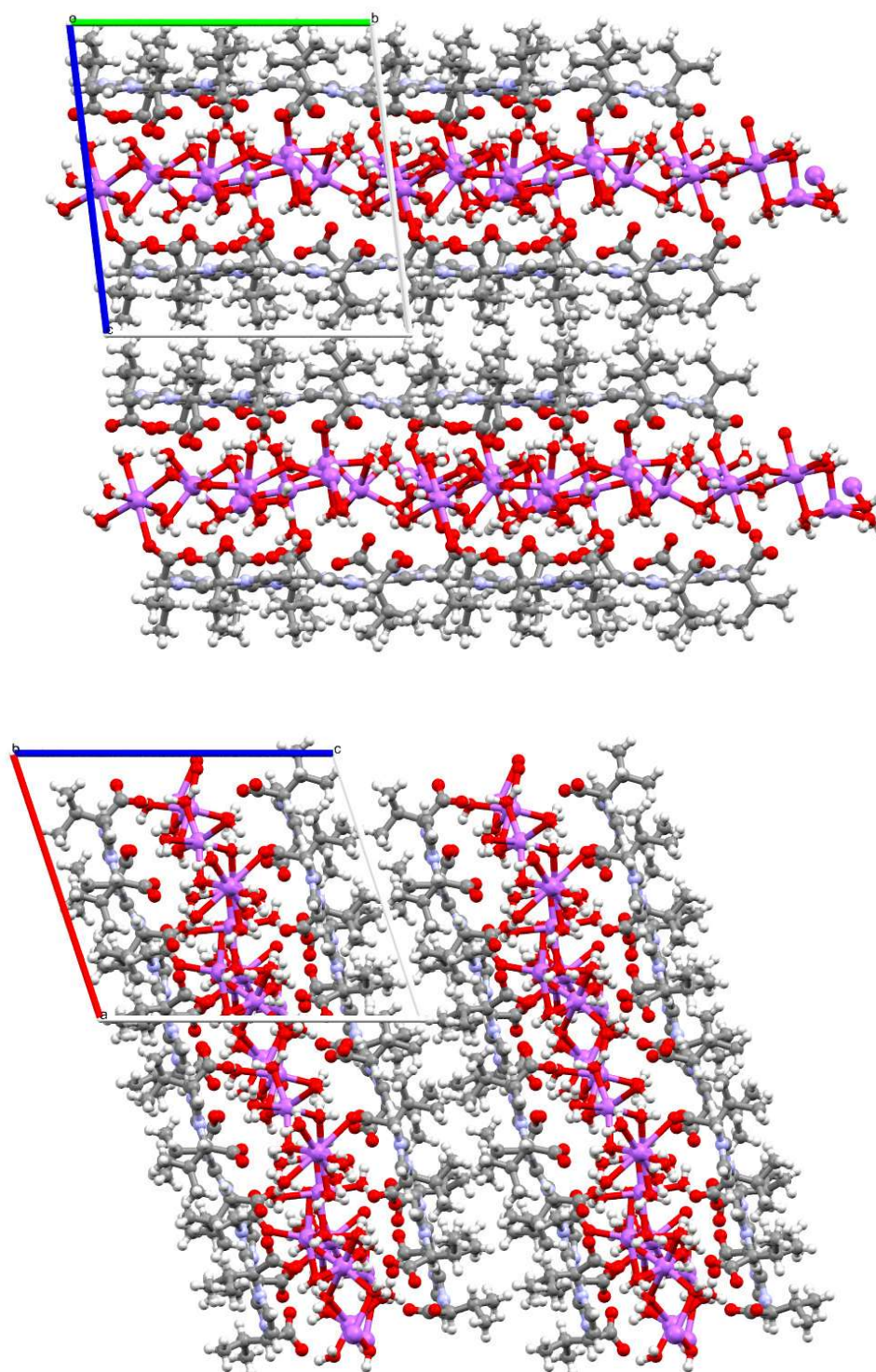
<sup>a</sup>  $[\alpha]_{\text{D}}$  determined in water at room temperature.



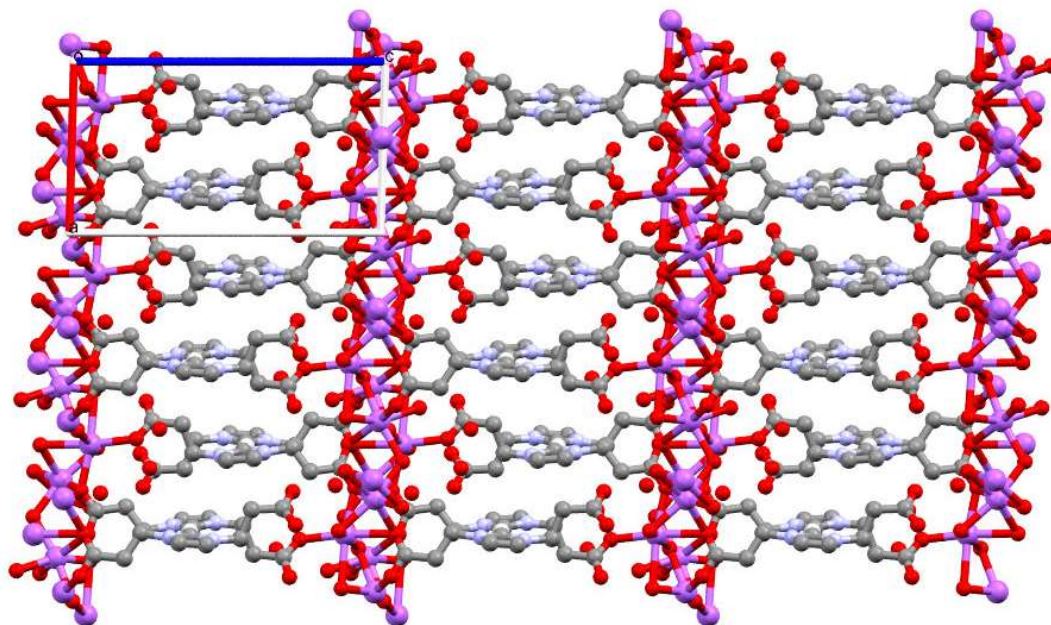
**Figure S7.** Crystal packing views of complex **1f**.



**Figure S8.** Crystal packing views of complex **2c**.

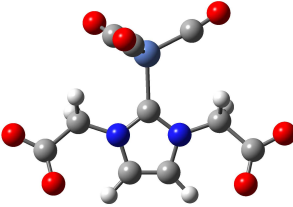
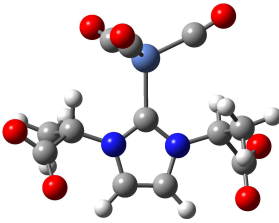
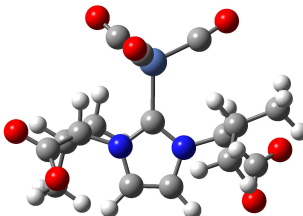
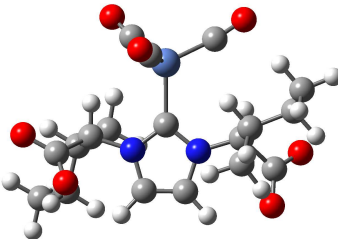


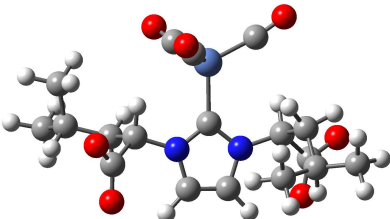
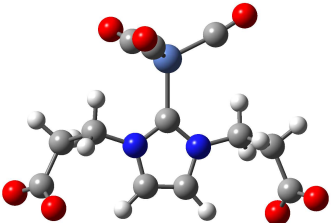
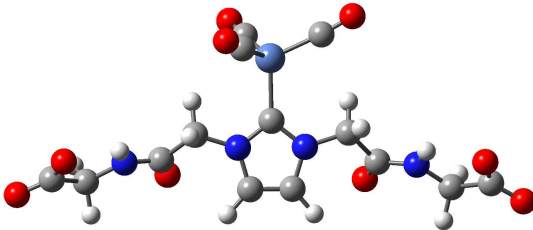
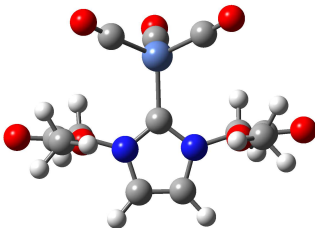
**Figure S9.** Crystal packing views of complex **2g** viewed along *b* axis.





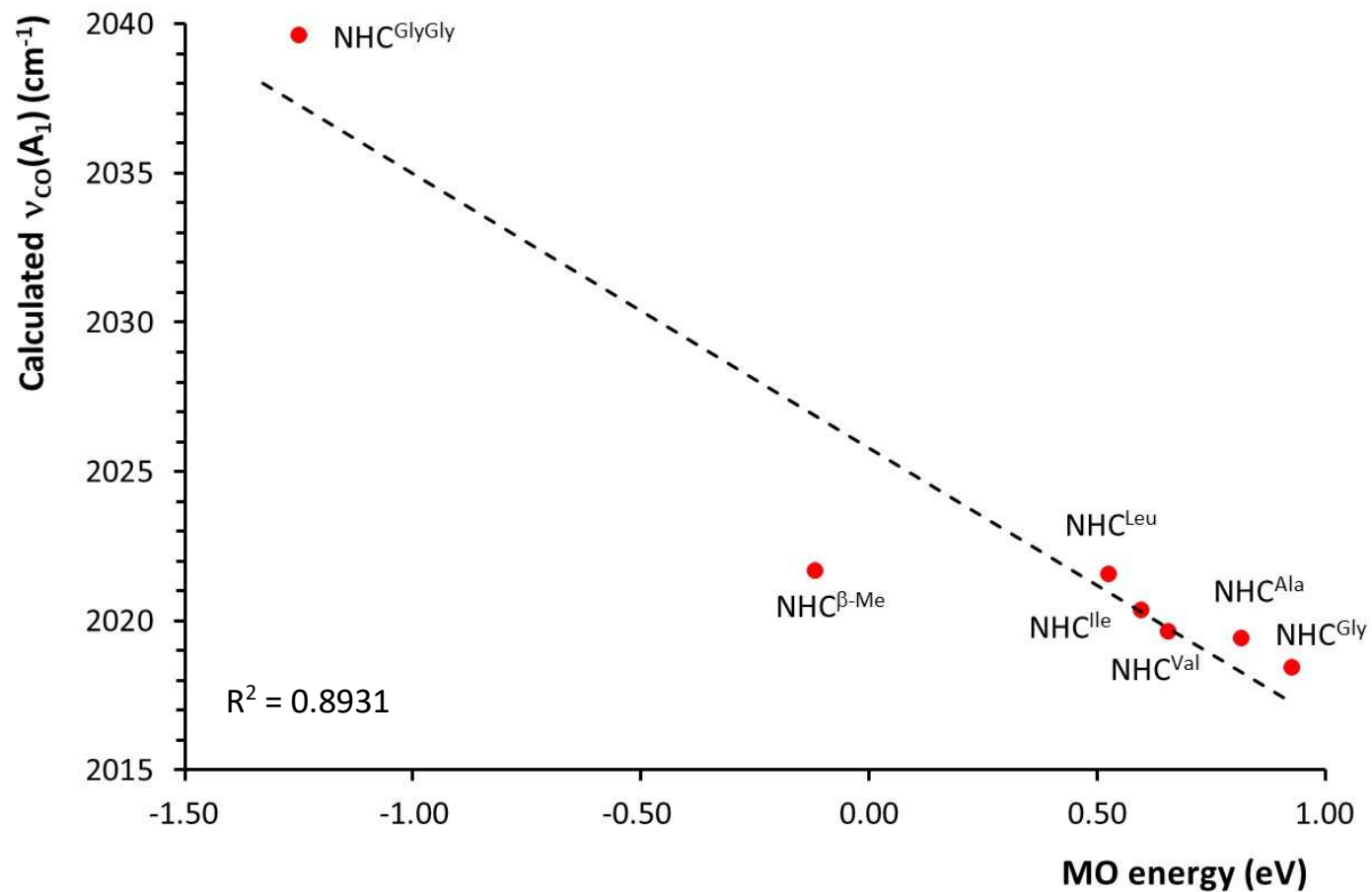
**Table S4.** Optimized structures of complexes  $[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{R}})]^{2-}$  and their calculated properties.

NHC	TEP ( $\text{cm}^{-1}$ )	Unscaled $\nu_{\text{CO}}$ ( $\text{Å}_1$ )	$d(\text{Ni-C})$ ( $\text{Å}$ )	Optimized structures <sup>a</sup>
$\text{NHC}^{\text{Gly}}$	2018.4	2115.5	2.008	
$\text{NHC}^{\text{Ala}}$	2019.4	2116.5	2.016	
$\text{NHC}^{\text{Val}}$	2019.6	2116.8	2.027	
$\text{NHC}^{\text{iLeu}}$	2020.3	2117.5	2.026	

NHC <sup>Leu</sup>	2021.5	2118.8	2.018	
NHC <sup><math>\beta</math>-Me</sup>	2021.6	2118.9	2.015	
NHC <sup>GlyGly</sup>	2039.6	2137.7	1.999	
Methyl diester of NHC <sup>Gly</sup>	2156.7	2057.7	1.985	

<sup>a</sup> The mPW1PW91 functional and the basis sets 6-311+G(2d) for Ni and 6-311+G(d,p) for all other atoms were used for calculations. Optimizations were carried out without symmetry restrictions, with tight option and the ultrafine integration grid.

**Figure S10.** Correlation between calculated TEP values ( $\nu_{\text{CO}}$ ) of the  $\text{NHC}^{\text{R}}$  carbenes and the MO energy of the  $\sigma$  lone pair orbitals.

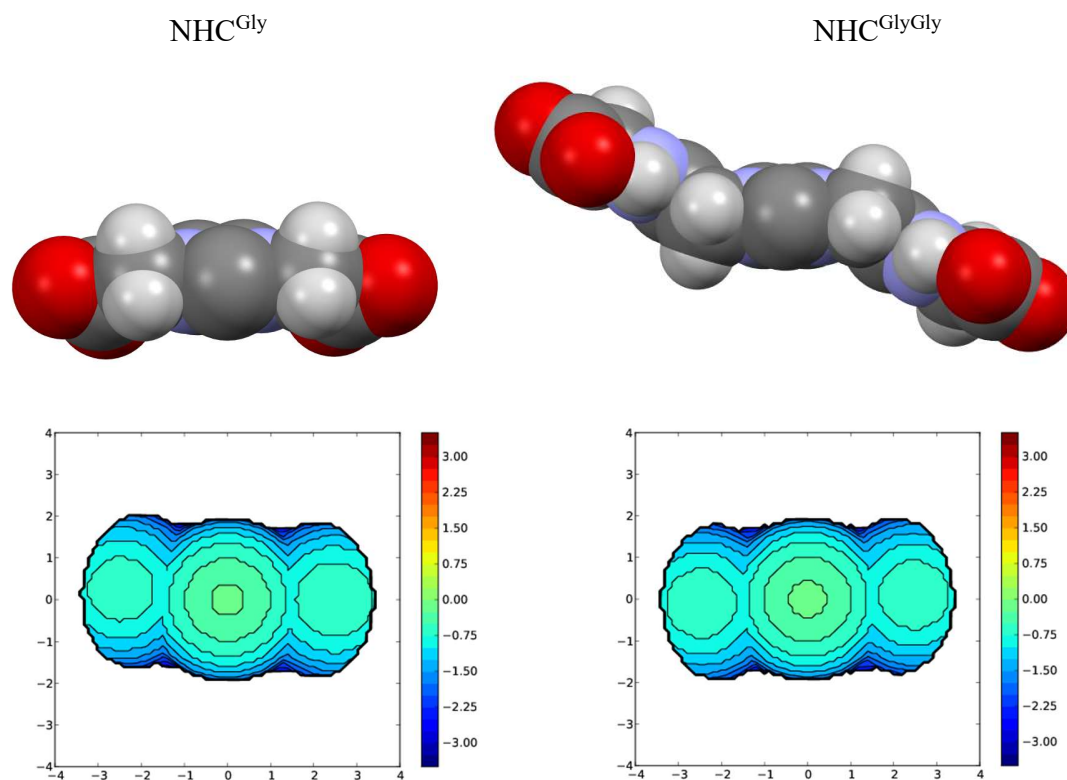


**Table S5.** Percent buried volume, % $V_{\text{bur}}$ , of  $\text{NHC}^{\text{R}}$  ligands.<sup>a</sup>

$\text{NHC}^{\text{R}}$	% $V_{\text{bur}}$		
	Determined from optimized $[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{R}})]^{2-}$	Determined from optimized $[\text{Ag}(\text{NHC}^{\text{R}})_2]^{3-}$	Determined from X-ray data
$\text{NHC}^{\text{Gly}}$	26.2	26.3	28.9
$\text{NHC}^{\text{Ala}}$	28.1	29.0	-
$\text{NHC}^{\text{Val}}$	30.0	30.2	37.8
$\text{NHC}^{\text{iLeu}}$	29.9	30.4	-
$\text{NHC}^{\text{Leu}}$	28.9	28.6	-
$\text{NHC}^{\beta\text{-Me}}$	26.2	26.2	27.3
$\text{NHC}^{\text{GlyGly}}$	26.1	26.2	-

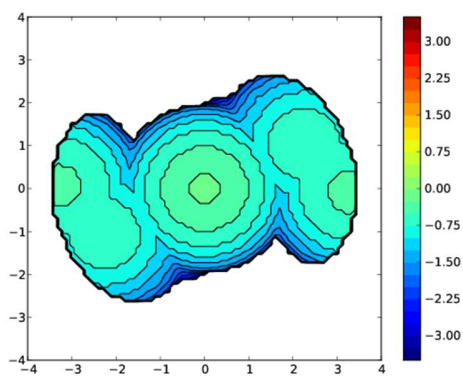
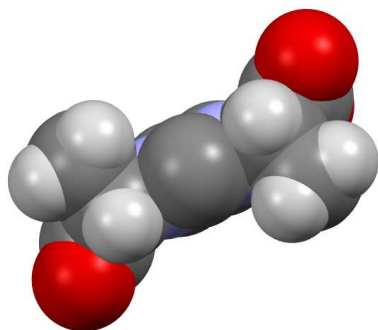
<sup>a</sup> Percentage buried volumes were calculated using the bond length for Ag–C fixed at 2 Å, a spherical radius of 3.5 Å, bond radii scaled by 1.17, and a mesh spacing of 0.10 (H atoms were excluded).

**Figure S11.** Selected steric maps from optimized  $[\text{Ag}(\text{NHC}^{\text{R}})_2]^{3-}$  complexes viewed along the Ag-C<sub>carbene</sub> vector.





NHC<sup>Ala</sup>



NHC<sup>Val</sup>

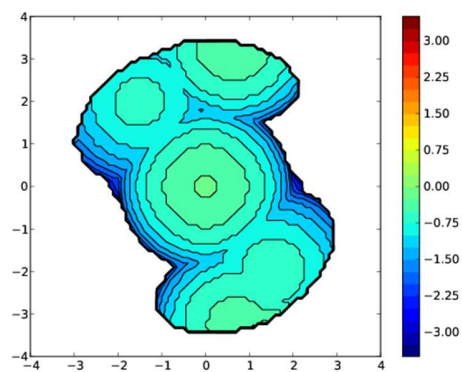
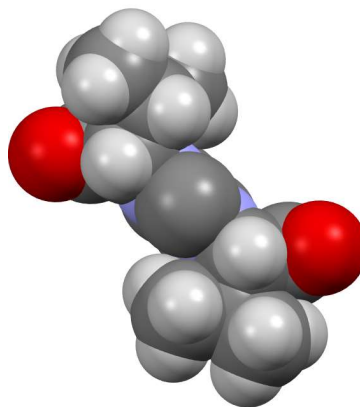
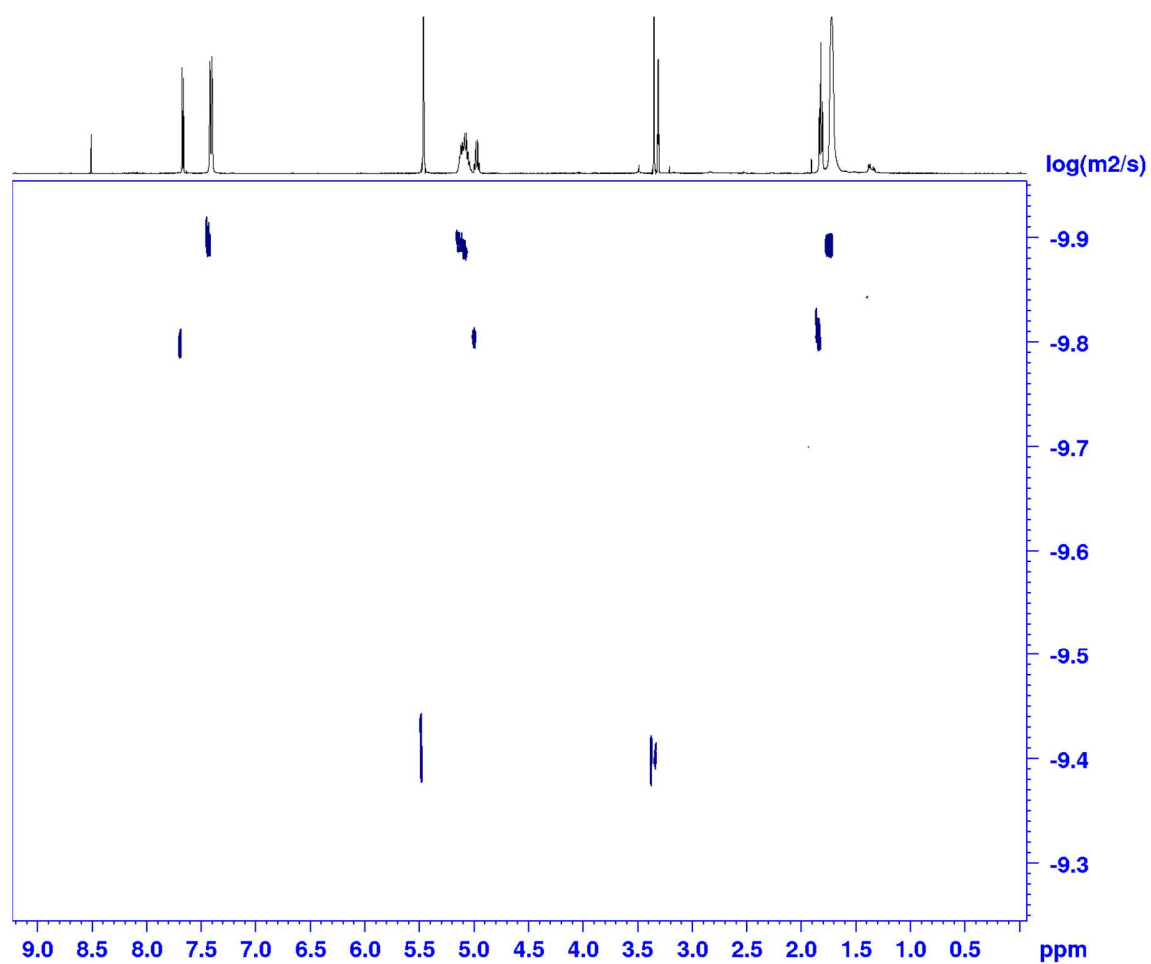
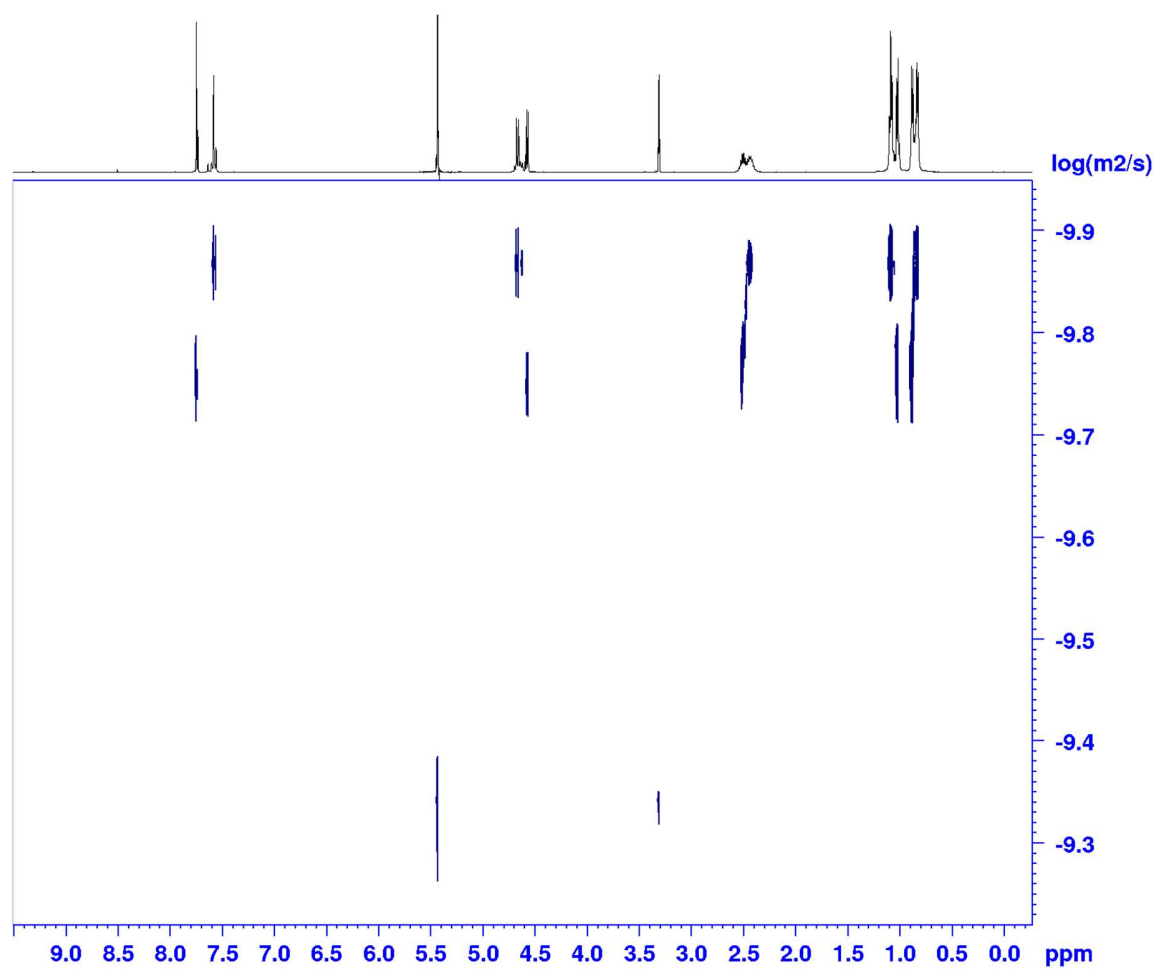


Figure S12.  $^1\text{H}$  DOSY NMR spectra of **2b-c**.

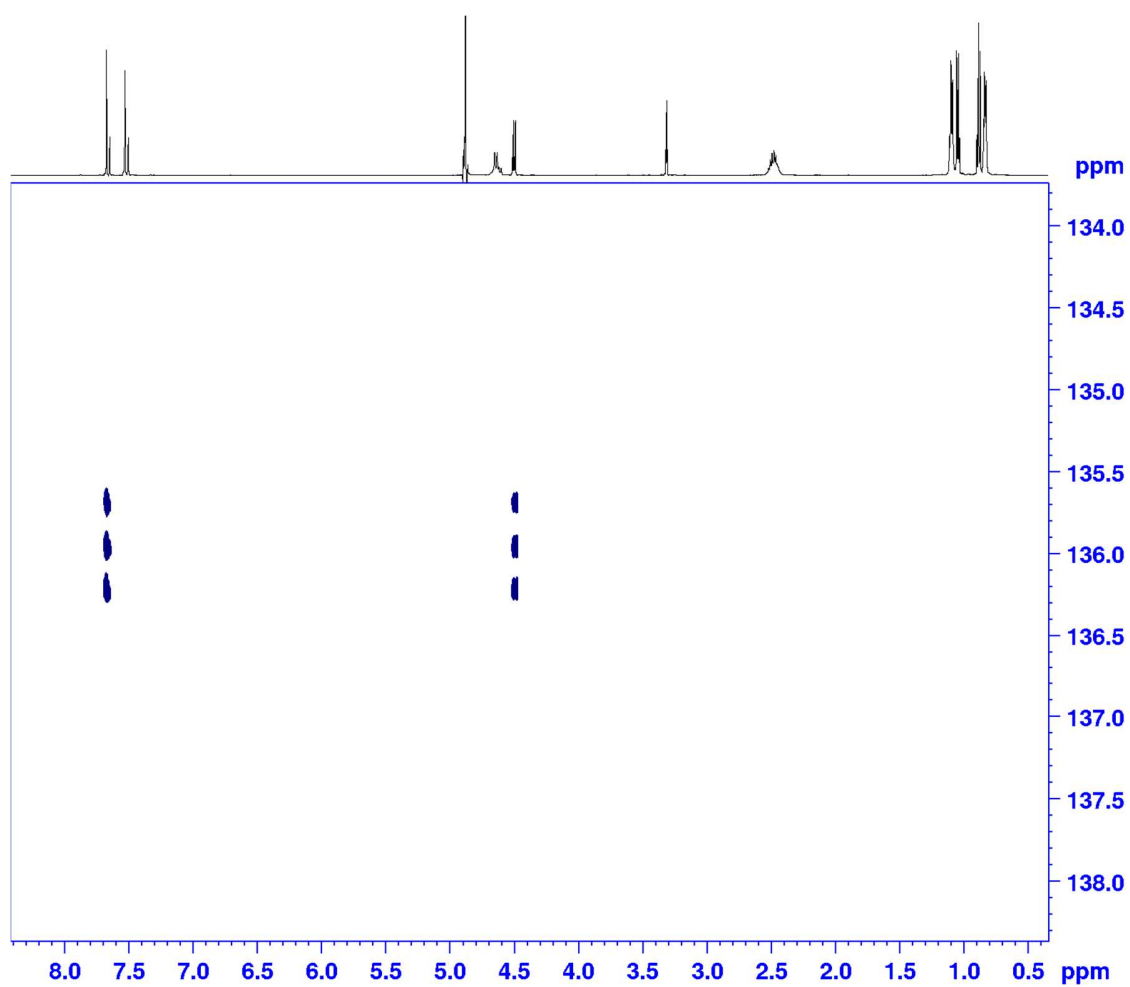
**2b**



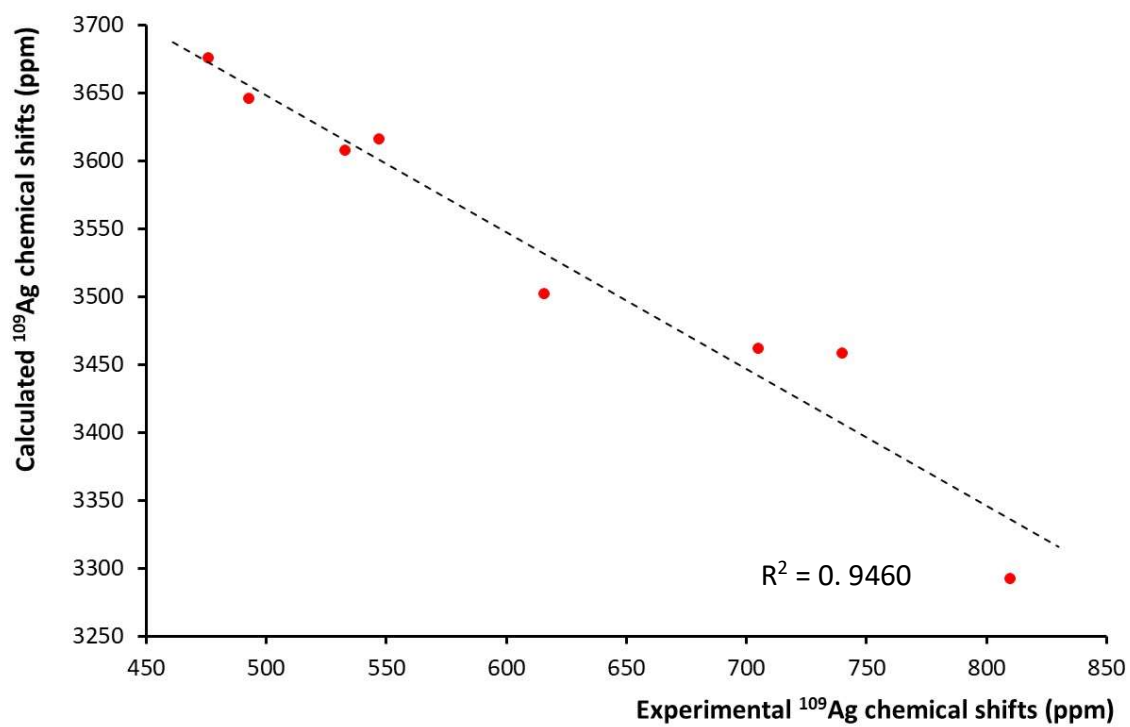
2c



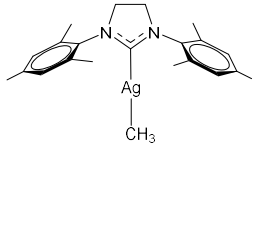
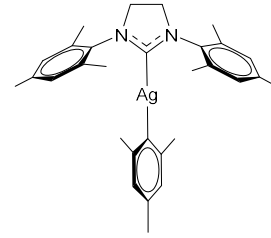
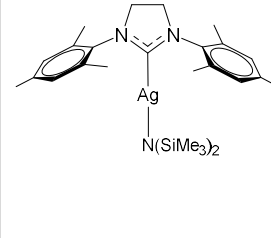
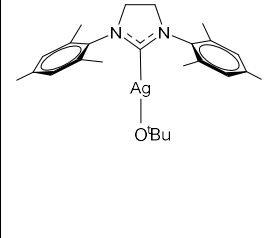
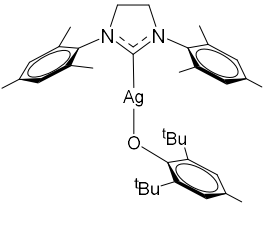
**Figure S13.** Band selective constant time  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR spectra (resolution enhanced by NUS) of **2c**.

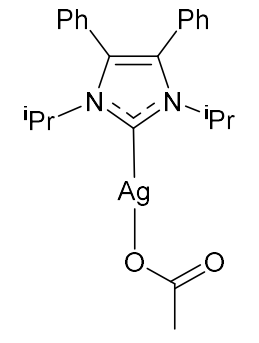
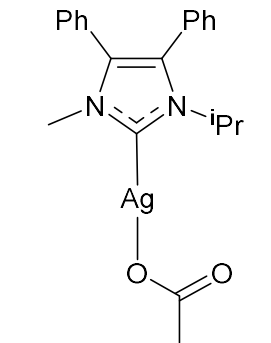
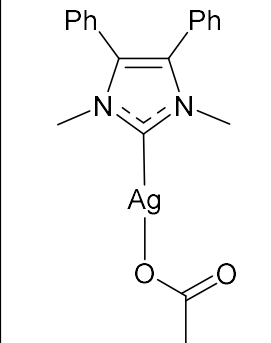


**Figure S14.** Correlation between calculated  $\sigma(^{109}\text{Ag})$  and experimental  $\delta(^{109}\text{Ag})$  chemical shifts for selected NHC silver complexes.



**Table S6.** Calculated  $\sigma(^{109}\text{Ag})$  and experimental  $\delta(^{109}\text{Ag})$  data for selected NHC silver complexes.

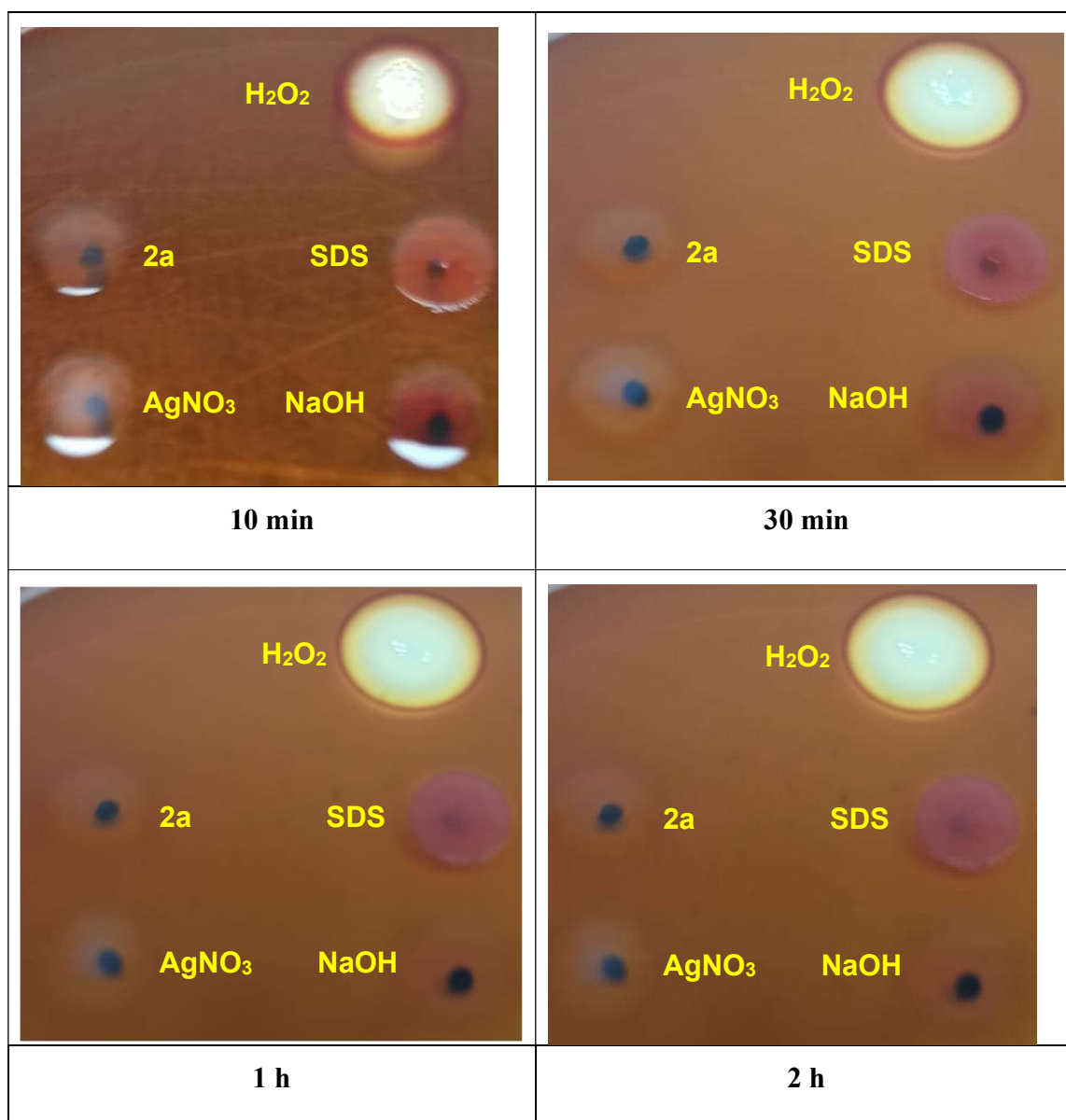
Complex					
$\delta_{\text{exp}}$	810	740	705	616	547
$\sigma_{\text{calc}}$	3292	3458	3462	3502	3616

Complex			
$\delta_{\text{exp}}$	533	493	476
$\sigma_{\text{calc}}$	3608	3646	3676

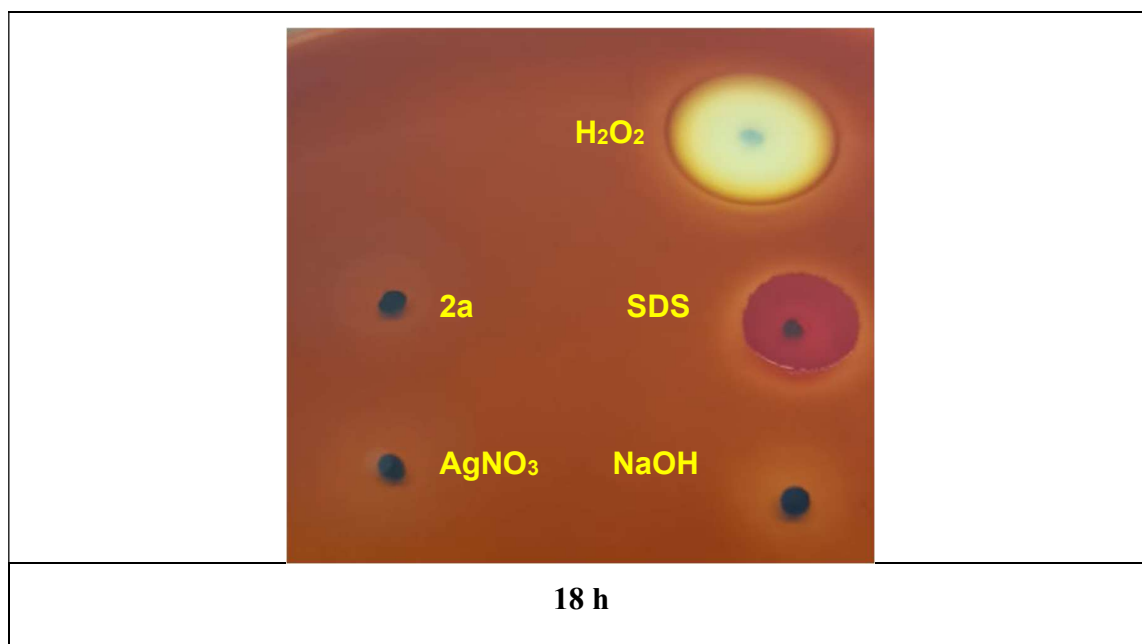
**Table S7.** Antimicrobial activities of complexes **2** evaluated by MIC and MBC ( $\mu\text{g/mL}$ ).

Complex	<i>E. coli</i>		<i>P. aeruginosa</i>		<i>S. Aureus</i>	
	MIC	MBC	MIC	MBC	MIC	MBC
<b>2a</b>	90.3	108.2	90.3	>216.4	90.3	144.4
<b>2b</b>	119.4	119.4	99.7	119.4	80.0	80.0
<b>2c</b>	189.3	212.7	189.3	212.7	165.2	212.7
<b>2c'</b>	141.8	141.8	141.8	141.8	141.8	165.2
<b>2e</b>	178.2	204.3	178.2	229.5	178.2	331.2
<b>2d</b>	204.3	229.5	229.5	229.5	204.3	229.5
<b>2f</b>	179.2	205.3	179.2	230.7	179.2	230.7
<b>2g</b>	139.1	159.4	119.4	179.1	119.4	277.6

**Figure S15.** Qualitative hemolysis test of complex **2a** and several control chemicals ( $\text{AgNO}_3$ ,  $\text{H}_2\text{O}_2$ , sodium dodecyl sulfate, SDS and  $\text{NaOH}$ ) for comparison.<sup>a</sup>







<sup>a</sup> Concentrations: **2a**, 10 mM; AgNO<sub>3</sub>, 10 mM; H<sub>2</sub>O<sub>2</sub>, 10 %; SDS 1 %; and NaOH 0.2 M.

**Table S8.** Crystal data and structure refinement for **1f**.

Empirical formula	$\text{C}_{11}\text{H}_{14}\text{N}_4\text{O}_6$	
Formula weight	298.26	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 9.0622(17)$ Å	$\alpha = 85.417(7)^\circ$
	$b = 10.8523(14)$ Å	$\beta = 82.590(10)^\circ$
	$c = 13.124(2)$ Å	$\gamma = 89.894(8)^\circ$
Volume	1275.8(4) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.553 Mg/m <sup>3</sup>	
Absorption coefficient	0.128 mm <sup>-1</sup>	
F(000)	624	
Crystal size	0.200 x 0.080 x 0.050 mm <sup>3</sup>	
Theta range for data collection	2.266 to 25.249°.	
Index ranges	$-10 \leq h \leq 10$ , $-11 \leq k \leq 13$ , $-15 \leq l \leq 15$	
Reflections collected	37232	
Independent reflections	4586 [R(int) = 0.1559]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.5847	
Refinement method	Full-matrix least-squares on $F^2$	
Data / restraints / parameters	4586 / 97 / 381	
Goodness-of-fit on $F^2$	1.162	
Final R indices [ $I > 2\sigma(I)$ ]	$R1 = 0.1386$ , $wR2 = 0.2881$	
R indices (all data)	$R1 = 0.1693$ , $wR2 = 0.3012$	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.973 and -0.515 e <sup>-</sup> Å <sup>-3</sup>	

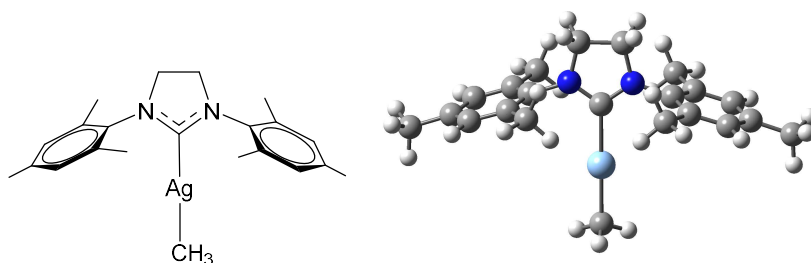
**Table S9.** Crystal data and structure refinement for **2c**.

Empirical formula	$\text{C}_{104}\text{H}_{224}\text{Ag}_4\text{N}_{16}\text{Na}_{12}\text{O}_{74}$	
Formula weight	3590.34	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	$a = 16.038(9)$ Å	$\alpha = 82.98(2)^\circ$
	$b = 17.017(7)$ Å	$\beta = 71.63(3)^\circ$
	$c = 18.571(10)$ Å	$\gamma = 88.37(2)^\circ$
Volume	$4774(4)$ Å <sup>3</sup>	
Z	1	
Density (calculated)	1.249 Mg/m <sup>3</sup>	
Absorption coefficient	0.513 mm <sup>-1</sup>	
F(000)	1872	
Crystal size	0.350 x 0.200 x 0.100 mm <sup>3</sup>	
Theta range for data collection	1.811 to 25.250 °	
Index ranges	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -22 ≤ l ≤ 22	
Reflections collected	170625	
Independent reflections	33843 [R(int) = 0.0867]	
Completeness to theta = 25.242°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6494	
Refinement method	Full-matrix least-squares on $F^2$	
Data / restraints / parameters	33843 / 447 / 1891	
Goodness-of-fit on $F^2$	1.059	
Final R indices [ $I > 2\sigma(I)$ ]	$R1 = 0.0708$ , $wR2 = 0.1964$	
R indices (all data)	$R1 = 0.0887$ , $wR2 = 0.2119$	
Absolute structure parameter	0.034(6)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.769 and -0.975 e·Å <sup>-3</sup>	

**Table S10.** Crystal data and structure refinement for **2g**.

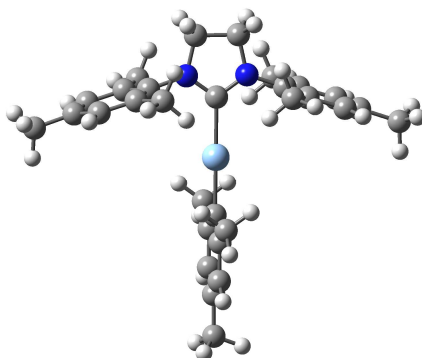
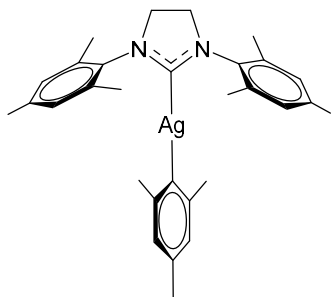
Empirical formula	$\text{C}_{18}\text{H}_{38}\text{AgN}_4\text{Na}_3\text{O}_{17}$	
Formula weight	759.36	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	$a = 8.6893(3)$ Å	$\alpha = 77.6730(10)^\circ$
	$b = 11.9503(4)$ Å	$\beta = 88.4700(10)^\circ$
	$c = 15.6733(4)$ Å	$\gamma = 75.6120(10)^\circ$
Volume	1539.52(8) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.638 mg/m <sup>3</sup>	
Absorption coefficient	0.776 mm <sup>-1</sup>	
F(000)	780	
Crystal size	0.500 x 0.400 x 0.200 mm <sup>3</sup>	
Theta range for data collection	1.997 to 25.246°	
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -17 ≤ l ≤ 18	
Reflections collected	31129	
Independent reflections	5521 [R(int) = 0.0426]	
Completeness to $\theta = 25.242^\circ$	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6266	
Refinement method	Full-matrix least-squares on $F^2$	
Data / restraints / parameters	5521 / 0 / 388	
Goodness-of-fit on $F^2$	1.087	
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0335, wR2 = 0.0884	
R indices (all data)	R1 = 0.0341, wR2 = 0.0888	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.671 and -0.761 e·Å <sup>-3</sup>	

**Table S11.** Coordinates and optimized structures of NHC-silver complexes used for the correlation between calculated and experimental  $^{109}\text{Ag}$  NMR chemical shifts.



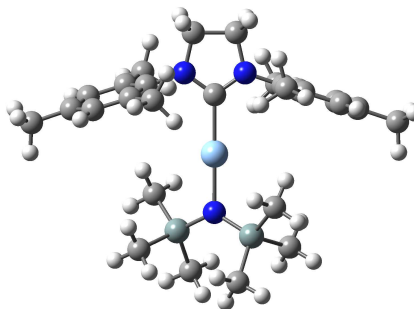
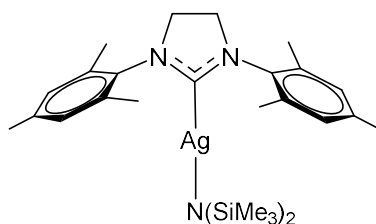
Ag	0.00007300	1.69883600	-0.00546000
N	1.08680900	-1.27546500	0.01150600
N	-1.08689100	-1.27544700	0.01146300
C	-0.00003500	-0.48907400	0.00532500
C	-0.76901400	-2.72394000	0.02223800
C	0.76890600	-2.72395100	0.02239200
C	2.44832100	-0.81673700	0.00490300
C	3.10150100	-0.62098000	-1.22115200
C	3.10806100	-0.60369700	1.22474400
C	4.43727300	-0.21775900	-1.20204700
C	4.44351500	-0.20083500	1.19275000
C	5.12628400	-0.00241100	-0.00801400
H	4.94964300	-0.05940100	-2.14719900
H	4.96099100	-0.02892900	2.13277300
C	-2.44839400	-0.81669000	0.00486300
C	-3.10819600	-0.60390200	1.22470600
C	-3.10150300	-0.62065700	-1.22119500
C	-4.44365000	-0.20101700	1.19272300
C	-4.43725900	-0.21740800	-1.20207800
C	-5.12634100	-0.00231400	-0.00803200
H	-4.96117800	-0.02931900	2.13275400
H	-4.94957200	-0.05882400	-2.14722400
C	2.37634800	-0.80035700	-2.53166600
H	3.04902100	-0.63284700	-3.37431300
H	1.95542600	-1.80448000	-2.64073200
H	1.54687600	-0.09338100	-2.61945800
C	6.55921900	0.47092000	-0.01455500
H	6.60965900	1.56500100	-0.00100800
H	7.10675300	0.11095100	0.85978400
H	7.09137400	0.13308200	-0.90687300
C	2.38970900	-0.76437600	2.54139600
H	1.56022700	-0.05667700	2.62312800
H	1.97010100	-1.76708200	2.66724300
H	3.06662600	-0.58416200	3.37801100
C	-2.37626900	-0.79975000	-2.53170300
H	-1.54681400	-0.09272900	-2.61930800
H	-1.95530800	-1.80383700	-2.64093900
H	-3.04890000	-0.63209600	-3.37435600
C	-6.55926500	0.47105000	-0.01459600
H	-7.10651200	0.11204400	0.86031400
H	-6.60967000	1.56514700	-0.00223400
H	-7.09173300	0.13226200	-0.90637100
C	-2.38993500	-0.76492700	2.54136400
H	-1.97060800	-1.76776800	2.66710700
H	-1.56026300	-0.05746700	2.62321700
H	-3.06683600	-0.58463600	3.37797500
H	1.19440600	-3.21371700	-0.85685500
H	1.19415300	-3.20044900	0.90901600
H	-1.19433900	-3.21357800	-0.85716700
H	-1.19445200	-3.20055100	0.90870600
C	0.00025600	3.82020600	-0.00953300

H	0.00153100	4.21571700	1.01184000
H	0.88455200	4.21512700	-0.52057400
H	-0.88519600	4.21530400	-0.51843100



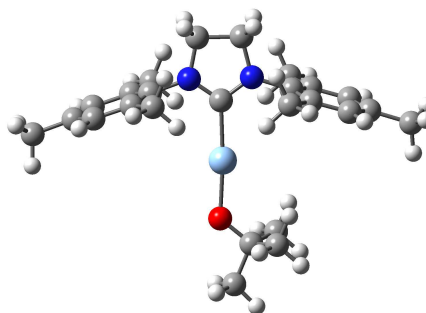
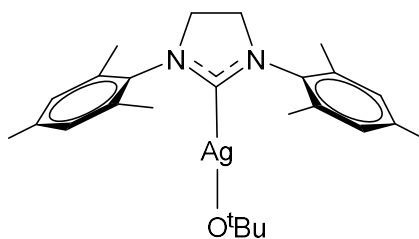
Ag	0.00131900	0.57341400	-0.01054300
N	1.08191200	-2.38556600	0.08088600
N	-1.09301600	-2.38035400	0.08151900
C	-0.00368300	-1.59911300	0.04214900
C	-0.77800400	-3.82768200	0.15249900
C	0.75998700	-3.83124200	0.15457600
C	2.44425900	-1.93071200	0.03331200
C	3.07925500	-1.79889000	-1.21073100
C	3.12224600	-1.65902600	1.23146600
C	4.41472800	-1.39425000	-1.23187400
C	4.45640500	-1.25753100	1.15878500
C	5.12070400	-1.11801300	-0.06074600
H	4.91301800	-1.28455600	-2.19122400
H	4.98826600	-1.03907700	2.08091200
C	-2.45311000	-1.91894500	0.03219400
C	-3.13326000	-1.65044300	1.22983200
C	-3.08391600	-1.77759100	-1.21294300
C	-4.46520200	-1.24198200	1.15548900
C	-4.41731500	-1.36628800	-1.23572700
C	-5.12528100	-1.09270200	-0.06517400
H	-4.99864700	-1.02578700	2.07723200
H	-4.91234100	-1.24922900	-2.19589600
C	2.33810500	-2.05093000	-2.50053000
H	2.99672500	-1.91563400	-3.35977300
H	1.93107300	-3.06528700	-2.55552700
H	1.49706100	-1.36148500	-2.61276200
C	6.55226900	-0.64363100	-0.11110300
H	6.60162600	0.45039800	-0.09722700
H	7.12675600	-1.00396700	0.74576900
H	7.05665800	-0.98007900	-1.01966500
C	2.42582800	-1.75879600	2.56589600
H	1.60197100	-1.04298300	2.63351100
H	2.00278700	-2.75250900	2.74147700
H	3.11848300	-1.54776200	3.38210100
C	-2.34046500	-2.02689500	-2.50193800
H	-1.49802100	-1.33850600	-2.61022300
H	-1.93498600	-3.04173300	-2.55910800
H	-2.99700800	-1.88779400	-3.36216500
C	-6.55432400	-0.61098100	-0.11722400
H	-7.13206500	-0.96963400	0.73814900
H	-6.59814400	0.48326500	-0.10191000
H	-7.05887300	-0.94355400	-1.02713600
C	-2.44152300	-1.76196800	2.56578300
H	-2.03330200	-2.76203000	2.74077500
H	-1.60776400	-1.05817700	2.63695100
H	-3.13324100	-1.54271900	3.38061100
H	1.18589100	-4.36000400	-0.70135600
H	1.18308600	-4.26890300	1.06188700

H	-1.20397800	-4.35211400	-0.70612300
H	-1.20557300	-4.26585400	1.05739500
C	0.00649500	2.70539800	-0.01799700
C	0.00834500	3.43693900	-1.22220100
C	0.00264500	3.43985700	1.18465300
C	0.00763500	4.83670300	-1.21299700
C	0.00195900	4.83946400	1.17252300
C	0.00714300	5.56058800	-0.02107100
H	0.00583100	5.37849700	-2.15804600
H	-0.00434300	5.38336100	2.11636700
C	0.00578000	2.72359600	-2.55966400
H	0.87939600	2.07115500	-2.66248100
H	-0.87992900	2.08863400	-2.66921800
H	0.01581400	3.42619000	-3.39848800
C	-0.00547400	2.73029700	2.52420600
H	-0.88766900	2.08964400	2.62887300
H	0.87192500	2.08426500	2.63589600
H	-0.00656200	3.43527700	3.36108300
C	0.04208500	7.07099000	-0.02222900
H	1.07082100	7.45102100	-0.01383300
H	-0.44506400	7.48485000	-0.90975100
H	-0.45983800	7.48650500	0.85631400



Ag	0.00005700	0.40005200	-0.00006600
N	1.08867500	-2.51472200	0.04340600
N	-1.08803100	-2.51491600	-0.04321600
C	0.00025300	-1.73201500	-0.00004200
C	-0.76500500	-3.96122900	-0.07110400
C	0.76587500	-3.96107800	0.07191300
C	2.44643400	-2.05436500	0.14553700
C	3.22243000	-1.95119200	-1.01937800
C	2.97883000	-1.74930500	1.40786500
C	4.54914400	-1.53708800	-0.89414800
C	4.31074600	-1.33957100	1.48072400
C	5.11231400	-1.22574200	0.34405000
H	5.15495900	-1.44501600	-1.79129600
H	4.73018000	-1.09645000	2.45311500
C	-2.44586500	-2.05481500	-0.14553800
C	-3.22208000	-1.95182100	1.01923700
C	-2.97810700	-1.74982600	-1.40796300
C	-4.54885300	-1.53793300	0.89377700
C	-4.31006700	-1.34031000	-1.48104400
C	-5.11185600	-1.22664300	-0.34449800
H	-5.15483200	-1.44596100	1.79082300
H	-4.72938000	-1.09724100	-2.45350200
C	2.64258400	-2.25072300	-2.37965500
H	3.35749600	-2.00795700	-3.16696200
H	2.37945800	-3.30766500	-2.49315700
H	1.73548400	-1.67019200	-2.56316100
C	6.53742600	-0.74113900	0.44766100
H	6.58409500	0.35054600	0.37397600
H	6.98938500	-1.02111700	1.40202100
H	7.16062400	-1.14728100	-0.35236100
C	2.13661300	-1.82498700	2.65726800

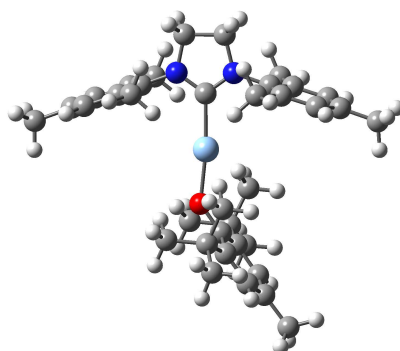
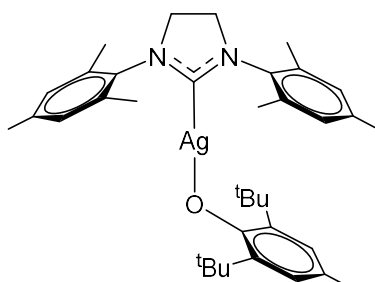
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H	2.74839400	-1.67318000	3.54779600
C	-2.13567700	-1.82538700	-2.65722800
H	-1.35803100	-1.05615400	-2.65356200
H	-1.63162700	-2.79039800	-2.76164600
H	-2.74742500	-1.67419900	-3.54788500
C	-6.53702000	-0.74225100	-0.44838700
H	-7.15994300	-1.14719900	0.35244700
H	-6.58370700	0.34954400	-0.37637200
H	-6.98927500	-1.02370000	-1.40218000
C	-2.64253100	-2.25147500	2.37961400
H	-2.38144400	-3.30886700	2.49378100
H	-1.73431400	-1.67255100	2.56260200
H	-3.35685700	-2.00684900	3.16687600
H	1.27033600	-4.48242000	-0.74375400
H	1.10455300	-4.40265400	1.01299500
H	-1.10361000	-4.40324800	-1.01200500
H	-1.26938700	-4.48229400	0.74478500
N	-0.00031700	2.50066300	0.00013400
Si	1.35452500	3.25593500	-0.74281200
Si	-1.35550400	3.25529200	0.74308800
C	0.89763200	4.80408400	-1.75198700
H	0.44900700	5.59203800	-1.13939500
H	1.78297200	5.23670400	-2.23170300
H	0.18157100	4.56234800	-2.54413700
C	-0.89954200	4.80413100	1.75162700
H	-0.18314000	4.56324900	2.54372900
H	-0.45169800	5.59225900	1.13869300
H	-1.78515900	5.23617000	2.23136000
C	2.68100100	3.79153000	0.51137200
H	2.28493100	4.52400400	1.22193700
H	3.03713000	2.93663600	1.09623500
H	3.55252400	4.24461000	0.02474400
C	2.21533500	2.08062100	-1.96502400
H	2.59996300	1.18060400	-1.47355600
H	1.52858600	1.75941100	-2.75542800
H	3.06646400	2.57173500	-2.45075800
C	-2.68253000	3.78952000	-0.51110700
H	-2.28700700	4.52188500	-1.22209200
H	-3.03822400	2.93413400	-1.09552200
H	-3.55426500	4.24230600	-0.02458500
C	-2.21535700	2.07982200	1.96581800
H	-2.59966200	1.17952900	1.47460000
H	-1.52822300	1.75907800	2.75607500
H	-3.06660100	2.57058500	2.45169900



Ag	0.01642900	1.02904600	-0.00328800
N	1.48911700	-1.69359200	0.00161200
N	-0.67024000	-1.98302500	-0.00296400
C	0.30537300	-1.06291900	-0.00171600
C	-0.16081900	-3.37436000	0.01177400
C	1.36399500	-3.17025900	-0.00703600
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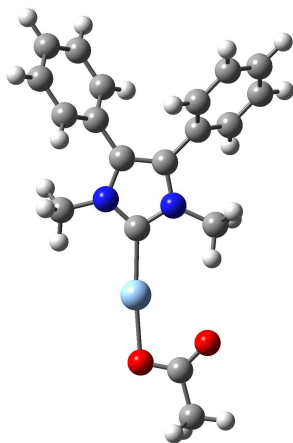
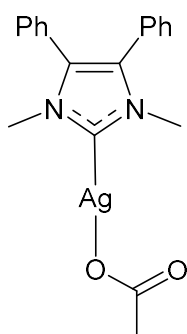


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C	4.65579300	-0.16097900	-1.19873800
C	4.66374100	-0.17623700	1.19654100
C	5.30906900	0.13344200	-0.00211500
H	5.13778800	0.08283100	-2.14142900
H	5.15280800	0.05627000	2.13867200
C	-2.07985100	-1.70502000	0.00234200
C	-2.74870300	-1.56919600	1.22772600
C	-2.76443000	-1.60972500	-1.21915500
C	-4.12649000	-1.34516500	1.20653000
C	-4.14105500	-1.38565900	-1.18845300
C	-4.84089800	-1.25137500	0.01195400
H	-4.65273900	-1.23305500	2.15043400
H	-4.67940000	-1.30511400	-2.12893400
C	2.69541300	-1.00992600	-2.53758500
H	3.35038600	-0.77284600	-3.37735900
H	2.38405700	-2.05308600	-2.64599100
H	1.79607600	-0.39494000	-2.63252700
C	6.66003500	0.80534100	0.00171900
H	6.55825400	1.88527700	0.15240200
H	7.29636200	0.42577800	0.80518200
H	7.18702100	0.65672500	-0.94323200
C	2.71246300	-1.04117900	2.53753300
H	1.80773300	-0.43557900	2.64087300
H	2.41138400	-2.08813500	2.63895000
H	3.36867900	-0.80471400	3.37650800
C	-2.03422100	-1.70578400	-2.53568600
H	-1.30160900	-0.90049800	-2.63757600
H	-1.49131300	-2.64979900	-2.64321600
H	-2.73034100	-1.63054500	-3.37235800
C	-6.32415900	-0.97403800	0.01346600
H	-6.79259300	-1.29186000	0.94753700
H	-6.52150300	0.09695300	-0.10234800
H	-6.83034900	-1.48662800	-0.80826600
C	-2.00317300	-1.62201300	2.53814300
H	-1.44212600	-2.55333100	2.66112100
H	-1.28399300	-0.80162100	2.61317700
H	-2.69159600	-1.53930700	3.38044800
H	1.83726800	-3.58561900	-0.90007700
H	1.86185300	-3.59956900	0.86540400
H	-0.52766400	-3.92326400	-0.85841400
H	-0.50894800	-3.89572800	0.90676600
O	-0.11466800	3.06481700	-0.00369300
C	-1.28018100	3.83114200	-0.00612200
C	-0.84854500	5.31299300	-0.00885400
H	-1.70213000	6.00072200	-0.01092200
H	-0.23743400	5.51924900	0.87383800
H	-0.23610100	5.51560000	-0.89146600
C	-2.12950700	3.54907600	-1.26524300
H	-2.44723900	2.50038200	-1.27563600
H	-3.02723700	4.17653800	-1.32185800
H	-1.52888200	3.72564400	-2.16223800
C	-2.13109200	3.55419900	1.25306200
H	-2.44907500	2.50563400	1.26721300
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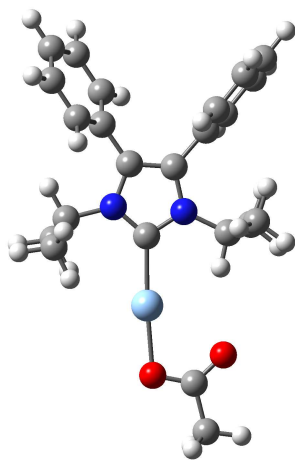
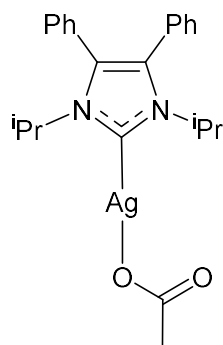
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C	-2.12320900	0.96038600	-0.00129400
C	-3.63045600	2.76854500	-0.00637300
C	-4.42636500	1.45111700	-0.00598800
C	-3.65071500	-0.97803600	0.00366000
C	-3.79945000	-1.65072100	-1.21858000
C	-3.80725600	-1.64318300	1.22968500
C	-4.11122200	-3.01082600	-1.18877200
C	-4.11910600	-3.00275500	1.20667000
C	-4.27346600	-3.70542500	0.01041600
H	-4.22052500	-3.54252700	-2.12982600
H	-4.23482000	-3.52853400	2.15039800
C	-1.12324200	3.21895200	-0.00818500
C	-0.60563700	3.67078000	1.21498600
C	-0.61195600	3.67389500	-1.23354500
C	0.43933000	4.59556000	1.18675100
C	0.43269500	4.59821100	-1.20881100
C	0.97337600	5.07034100	-0.01162800
H	0.85197600	4.94682300	2.12833900
H	0.84052800	4.95176000	-2.15174400
C	-3.59617600	-0.94323800	-2.53572400
H	-3.80035900	-1.61364500	-3.37163800
H	-4.24943300	-0.07239900	-2.64524800
H	-2.56752000	-0.58758200	-2.63993300
C	-4.56998000	-5.18458500	0.01632100
H	-3.64497600	-5.76654400	0.08677400
H	-5.19549000	-5.46659500	0.86658400
H	-5.08165300	-5.49676300	-0.89669800
C	-3.61137300	-0.92696600	2.54320600
H	-2.58339800	-0.57024300	2.65043200
H	-4.26548500	-0.05564800	2.64360400
H	-3.81972400	-1.59196400	3.38241400
C	-1.14540900	3.15909200	-2.54762300
H	-0.96585000	2.08581900	-2.65435100
H	-2.22338500	3.31652500	-2.64979400
H	-0.65978800	3.65971000	-3.38635200
C	2.13107400	6.03764800	-0.01532200
H	2.15813400	6.63785900	0.89681300
H	3.08443400	5.50284300	-0.08164400
H	2.08327300	6.72060300	-0.86686400
C	-1.13091500	3.15272800	2.53104600
H	-2.21121300	3.29284400	2.63274400
H	-0.93382900	2.08285700	2.64153700
H	-0.65306600	3.66392600	3.36786500
H	-5.05559100	1.33398500	-0.89116100
H	-5.06237700	1.33851800	0.87483500
H	-3.82349700	3.38219600	-0.88899400
H	-3.82253200	3.38201300	0.87671100
O	1.31572700	-1.43342300	0.00989200
C	2.64102000	-1.34239600	0.00357900
C	3.36784000	-1.34889000	-1.23343300
C	3.37787400	-1.32861900	1.23447800
C	4.76075200	-1.25585600	-1.19556400

C	4.77046500	-1.23620400	1.18374700
C	5.48568300	-1.18026400	-0.00935700
H	5.32011800	-1.25019200	-2.12418000
H	5.33733800	-1.21499600	2.10751300
C	2.66691300	-1.43442900	2.60546800
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C	1.72667000	-2.72096800	-2.61010400
H	1.19421000	-2.79263800	-3.56632400
H	2.32142400	-3.63212800	-2.49204100
H	1.00436000	-2.68412100	-1.79840500
C	1.82534700	-0.20169400	-2.89356300
H	1.07483800	-0.01603200	-2.12433200
H	2.47844500	0.67490200	-2.94074100
H	1.30684100	-0.28848200	-3.85602800
C	3.62841700	-1.64400300	-3.77470900
H	3.06208000	-1.77773600	-4.70165600
H	4.27204500	-0.77069700	-3.91254700
H	4.26850700	-2.52180700	-3.65247300
C	1.84741600	-0.15525100	2.88758300
H	2.49965000	0.72284300	2.91441200
H	1.09032200	0.01639800	2.12160600
H	1.33710700	-0.22636400	3.85569000
C	1.74917500	-2.67878200	2.64708700
H	1.01917600	-2.65462200	1.84181900
H	2.34341000	-3.59130200	2.53730400
H	1.22589200	-2.73596900	3.60933100
C	3.65939700	-1.58045000	3.77811500
H	4.30366900	-0.70459500	3.89491800
H	3.10079900	-1.69792400	4.71193500
H	4.29893200	-2.46007900	3.66631600
C	6.98991400	-1.03712600	-0.01675500
H	7.44239000	-1.48933600	0.87098400
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H	7.30503900	0.01414800	-0.03489400



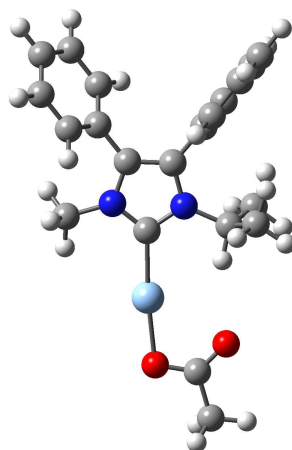
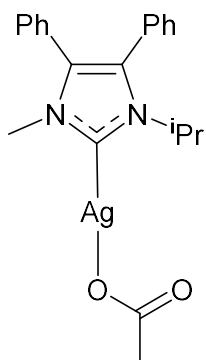
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C	0.72990700	-0.44155500	-0.07987500
C	-1.27204900	0.62790600	-0.00832100
C	-1.52513100	-0.71843900	-0.04107000
O	4.98455700	-0.72105300	-0.07498900
C	0.84436600	2.03653000	0.05009400
H	1.89576000	1.83094900	0.24496800
H	0.76278700	2.58564100	-0.88832500
H	0.43366500	2.64460500	0.85589600
C	-0.05744900	-2.78619200	-0.18924900
H	0.96757500	-2.94580600	-0.51521900
H	-0.20327100	-3.27606100	0.77470300

H	-0.74415700	-3.21895500	-0.91625700
C	5.33085700	0.50189700	0.13653700
C	6.83577100	0.73942700	0.19079800
H	7.29479500	0.42476800	-0.75005600
H	7.05661500	1.79058200	0.37300600
H	7.27905200	0.12809000	0.98113900
O	4.54059900	1.44571000	0.28998900
C	-2.21712900	1.75820000	0.06513100
C	-2.21109600	2.77318200	-0.90248500
C	-3.15647300	1.82263000	1.10320900
C	-3.11702300	3.82700600	-0.82929300
H	-1.50748700	2.72705900	-1.72677200
C	-4.06494400	2.87475300	1.17158100
H	-3.16803200	1.04570000	1.85951900
C	-4.04626100	3.88090500	0.20796100
H	-3.10065000	4.60344600	-1.58706400
H	-4.78459800	2.91093200	1.98282400
H	-4.75235100	4.70282300	0.26419800
C	-2.81403100	-1.43444900	-0.05656900
C	-3.11364300	-2.40904500	0.90657700
C	-3.77449800	-1.13535700	-1.03271400
C	-4.33817100	-3.07022500	0.88930900
H	-2.39373300	-2.63421300	1.68639600
C	-5.00063100	-1.79362800	-1.04461200
H	-3.55343400	-0.38588600	-1.78436300
C	-5.28488900	-2.76472000	-0.08659400
H	-4.55586600	-3.81880200	1.64408000
H	-5.73303900	-1.55057300	-1.80737200
H	-6.23997100	-3.27943300	-0.09880200



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N	-0.03825000	0.81109300	-0.00306500
C	-0.65517000	-0.39796500	0.01819300
C	1.35321600	0.65491000	0.01386500
C	1.59057500	-0.69194200	0.03453800
O	-4.91959900	-0.65067700	0.01589200
C	-0.82324100	2.07905900	-0.08311900
H	-1.85502900	1.73873700	-0.18060700
C	0.12508700	-2.78318300	0.15070900
H	1.12896400	-3.20782100	0.16523100
C	-5.29190100	0.58091300	-0.06600200
C	-6.80246000	0.78892900	-0.08349000
H	-7.24562300	0.36530700	0.82152000
H	-7.04821600	1.84820600	-0.15072400
H	-7.23992200	0.25571800	-0.93157700
O	-4.52324300	1.55142400	-0.12823200
C	2.36834000	1.73669400	-0.02248200

C	2.72082000	2.43827500	1.13722000
C	3.04197800	2.02799800	-1.21510400
C	3.70719100	3.42082500	1.10071600
H	2.22501800	2.20634800	2.07365300
C	4.03003100	3.00849100	-1.25152300
H	2.78544900	1.48321100	-2.11733800
C	4.36187500	3.71021600	-0.09465600
H	3.96809900	3.95550700	2.00823700
H	4.54096100	3.22315400	-2.18441700
H	5.13109900	4.47502800	-0.12291200
C	2.88642400	-1.40202100	0.02113500
C	3.24386600	-2.22681400	-1.05582500
C	3.79505400	-1.24239100	1.07480600
C	4.47290400	-2.87927200	-1.07322700
H	2.56022500	-2.34381600	-1.89071600
C	5.02754500	-1.89016600	1.05306100
H	3.53095000	-0.60797900	1.91343400
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H	4.73470700	-3.51147700	-1.91543800
H	5.72060100	-1.75386500	1.87678800
H	6.32807700	-3.21855000	-0.03330800
C	-0.61234900	-3.33436800	-1.07093600
H	-1.63482100	-2.95572500	-1.12592700
H	-0.10101000	-3.06477700	-1.99824000
H	-0.65843200	-4.42481400	-1.01272000
C	-0.55899600	-3.14380800	1.47137000
H	-0.00636600	-2.73976200	2.32280400
H	-1.57972300	-2.75886600	1.51156800
H	-0.60153900	-4.23073400	1.57921000
C	-0.73904000	2.89879600	1.20517300
H	-0.93974000	2.27391700	2.07856100
H	0.23020800	3.38368100	1.32998000
H	-1.50492600	3.67705800	1.17619000
C	-0.48343500	2.88657000	-1.33608500
H	0.51356900	3.32766400	-1.29474400
H	-0.55546800	2.26571500	-2.23231600
H	-1.20775900	3.69801700	-1.43739500



Ag	2.79602500	-0.89705400	-0.04875000
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N	0.09220100	0.60451000	-0.00027600
C	0.68926300	-0.61407100	-0.03838600
C	-1.30240900	0.47030800	-0.01260900
C	-1.56218000	-0.87295600	-0.04720200
O	4.93624500	-0.99584500	-0.05473200
C	0.90396100	1.85490400	0.09093000
H	1.92916600	1.49105500	0.17487600
C	5.33044400	0.22776600	0.03854000

C	6.84439100	0.40962700	0.04989700
H	7.27642200	-0.01746300	-0.85880700
H	7.10829900	1.46427700	0.12114000
H	7.27628200	-0.13477100	0.89375900
O	4.57969900	1.21155500	0.11610600
C	-2.29971000	1.56751700	0.03771900
C	-2.63913500	2.29243200	-1.11144400
C	-2.97075800	1.84944000	1.23402500
C	-3.61096700	3.28864100	-1.06068600
H	-2.14531200	2.06749700	-2.05058600
C	-3.94416200	2.84385300	1.28441900
H	-2.72411800	1.28618700	2.12763200
C	-4.26343400	3.56851900	0.13823500
H	-3.86244300	3.84151700	-1.95989700
H	-4.45355400	3.05127300	2.21975500
H	-5.02128000	4.34410700	0.17743000
C	-2.85504700	-1.58512800	-0.05468700
C	-3.18728000	-2.47836500	0.97411200
C	-3.78096200	-1.37012600	-1.08367400
C	-4.41001600	-3.14255500	0.96985600
H	-2.49321500	-2.63631500	1.79322500
C	-5.00621400	-2.03135900	-1.08384400
H	-3.53522500	-0.68385100	-1.88617800
C	-5.32274100	-2.92126700	-0.05993000
H	-4.65344700	-3.82704700	1.77590300
H	-5.71264800	-1.85296000	-1.88791000
H	-6.27694500	-3.43780500	-0.06217900
C	0.82680100	2.69535400	-1.18428400
H	1.00666300	2.07939500	-2.06845800
H	-0.13222900	3.20375400	-1.29387900
H	1.61009000	3.45586800	-1.15010100
C	0.58890700	2.64888500	1.35878800
H	-0.40169700	3.10560100	1.33330000
H	0.65952100	2.01331700	2.24471100
H	1.32636500	3.44766400	1.46552600
C	-0.11847900	-2.95477800	-0.15629900
H	0.92503300	-3.13077400	-0.40671200
H	-0.34490800	-3.44443700	0.79188100
H	-0.75696800	-3.37461100	-0.93359400

**Table S12.** Coordinates of complexes  $[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{R}})]^{2-}$  used for the determination of the Tolman Electronic Parameter (TEP).

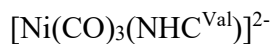
$[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{Gly}})]^{2-}$

Ni	-0.03544600	1.64388100	0.06741900
C	-0.52967200	1.94526200	1.75782600
C	1.53055500	2.44085100	-0.27517900
C	-1.18390600	2.26711900	-1.15458200
O	-0.82239000	2.14242500	2.85034200
O	-1.86697500	2.71641400	-1.96113800
O	2.46882500	3.06208000	-0.50419700
C	0.72224400	-2.48298000	-0.39372600
C	-0.63071100	-2.49123500	-0.41967200
H	1.46488100	-3.26138900	-0.41134000
H	-1.35608000	-3.28424100	-0.45700900
C	0.02648500	-0.35434000	-0.11651700
N	1.10922800	-1.17210900	-0.19687100
N	-1.04135200	-1.18635500	-0.23851000
C	2.49645600	-0.69850500	-0.17638300
H	2.70821000	-0.20341800	-1.12653300
H	2.56804000	0.06315000	0.59876400
C	-2.43274800	-0.73649000	-0.29944200
H	-2.51873400	0.13825000	0.34248800
H	-2.64858600	-0.40299200	-1.31814300
C	3.67068700	-1.70510200	0.07145800
C	-3.58343700	-1.72158000	0.09603000
O	4.77485000	-1.13348700	-0.02107100
O	3.41946700	-2.89829600	0.32516400
O	-3.30005800	-2.87577400	0.46614100
O	-4.70073400	-1.18170900	-0.03113700

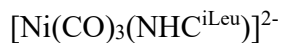
$[\text{Ni}(\text{CO})_3(\text{NHC}^{\text{Ala}})]^{2-}$

Ni	0.08663200	1.68397600	-0.00067600
C	1.06864900	2.07594500	-1.44739200
C	-1.47149300	2.54025100	-0.19985800
C	0.80677200	2.21160800	1.54828300
O	1.63908900	2.36852900	-2.39825500
O	1.22755800	2.59543600	2.54593200
O	-2.39364400	3.21025100	-0.34433000
C	-0.80424000	-2.45542000	-0.07346700
C	0.54225200	-2.50729000	0.03422100
H	-1.57143800	-3.20711800	-0.15252400
H	1.24527300	-3.32007900	0.00722100
C	-0.05116200	-0.32746200	0.03600100
N	-1.15299300	-1.11847100	-0.06209000
N	0.98906500	-1.20299000	0.09565100
C	-2.53067900	-0.62716600	-0.21376100
H	-2.56412700	0.32290800	0.31231800
C	2.38121600	-0.82646300	0.36625900
H	2.45871500	0.22526400	0.09932300
C	-3.61799400	-1.55443100	0.44242800
C	3.48764000	-1.59158800	-0.44584900
O	-3.68022200	-2.72527700	0.00482300
O	-4.34112700	-0.99333000	1.28637300
O	3.21598500	-2.72220500	-0.89421700
O	4.56508200	-0.96368300	-0.48460800
C	-2.84917800	-0.42819700	-1.69121500
H	-2.11659100	0.23349800	-2.16198900
H	-2.84472900	-1.39460800	-2.19989400
H	-3.84468400	0.01164600	-1.79757300
C	2.67653100	-0.98442400	1.85786400

H	3.69375500	-0.64257600	2.05497100
H	1.97454900	-0.40477400	2.46343800
H	2.59941700	-2.03520300	2.15188000



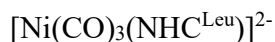
Ni	0.02048500	1.84045800	-0.02349800
C	-0.00580600	2.18064400	1.73544600
C	1.49399000	2.52379700	-0.77741100
C	-1.32324300	2.68237100	-0.85048300
O	-0.00760900	2.41848600	2.85685800
O	-2.11045400	3.34058400	-1.36848900
O	2.36981700	3.10131900	-1.24460300
C	0.49684200	-2.36751500	0.02848800
C	-0.84149800	-2.29128500	0.19418200
H	1.19750600	-3.18485000	0.00467800
H	-1.57333500	-3.03648800	0.44162600
C	-0.08176100	-0.18277900	-0.09020500
N	0.94851300	-1.07329900	-0.14627200
N	-1.18545900	-0.95796800	0.10825900
C	2.36317600	-0.71174000	-0.32328900
H	2.35961000	0.17563400	-0.95157100
C	-2.56544400	-0.47509800	0.12667800
H	-2.48589900	0.60780600	0.20383000
C	3.22070200	-1.78196800	-1.09444100
C	-3.43292500	-0.95136500	1.34855700
O	3.20559800	-2.95315400	-0.65209200
O	3.88274100	-1.31578200	-2.04023500
O	-3.01961500	-1.91239200	2.02179600
O	-4.49450900	-0.30278200	1.45715500
C	3.00394500	-0.32990500	1.02923500
H	2.40487500	0.50663300	1.41058400
C	-3.33012000	-0.79340900	-1.18292500
H	-4.24151500	-0.19574100	-1.08559300
C	-3.76104500	-2.25519600	-1.31029100
H	-2.90247400	-2.91067100	-1.48197400
H	-4.27951600	-2.59511700	-0.41160000
H	-4.43840600	-2.37184500	-2.16422500
C	-2.57746200	-0.35469700	-2.43558200
H	-3.18579900	-0.53728900	-3.32913400
H	-2.32641500	0.70642300	-2.40879900
H	-1.64202400	-0.90971900	-2.54977300
C	4.43103900	0.17096300	0.81633900
H	5.07320500	-0.63088600	0.44270600
H	4.46457900	0.98064600	0.08334300
H	4.84905500	0.53991100	1.75963300
C	2.96589900	-1.44551200	2.07060200
H	3.51077500	-2.32202700	1.71346300
H	3.41475300	-1.09677000	3.00792100
H	1.94057600	-1.75367800	2.28639800



Ni	0.28990800	1.85492000	-0.26055500
C	0.49030400	2.39327100	1.43739400
C	1.76675500	2.21675300	-1.20584800
C	-0.99534000	2.78947900	-1.08026700
O	0.64091700	2.75492800	2.51440700
O	-1.72968600	3.49237200	-1.61690000
O	2.66934200	2.59887400	-1.80445400
C	0.15430800	-2.34705900	0.25628900
C	-1.12537300	-2.04052600	0.56044900
H	0.71886100	-3.26404200	0.25401700
H	-1.91988600	-2.63282000	0.97266200
C	-0.10877800	-0.12159000	-0.06114800

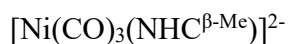


N	0.76428200	-1.16655100	-0.12312900
N	-1.27857600	-0.68565700	0.35254300
C	2.18050200	-1.05551600	-0.50260700
H	2.22198400	-0.25275700	-1.23484900
C	-2.55873100	0.00990000	0.47199900
H	-2.31633300	1.06717500	0.37876800
C	2.76597900	-2.32614300	-1.22290800
C	-3.29415300	-0.16388500	1.85087100
O	2.64077200	-3.42473200	-0.63562000
O	3.35717200	-2.07657800	-2.28984300
O	-2.91519000	-1.07797700	2.60473800
O	-4.23523200	0.64485600	1.99149700
C	3.04404700	-0.63422700	0.70804500
H	2.63684400	0.33219500	1.03554200
C	-3.54430700	-0.34233500	-0.67126800
H	-4.34098700	0.39802800	-0.54128800
C	-4.19448600	-1.72591400	-0.52340400
H	-3.48510700	-2.49923500	-0.83947800
H	-4.40714000	-1.90716100	0.53363300
C	-2.91878300	-0.16878400	-2.05293000
H	-3.65073000	-0.35496500	-2.84563300
H	-2.53095600	0.84101000	-2.19245400
H	-2.08519900	-0.86217100	-2.19618800
C	4.48967800	-0.40091100	0.25418700
H	4.94822000	-1.36609000	0.01522200
H	4.47676400	0.15675000	-0.68704900
C	2.95629300	-1.60464500	1.88381100
H	3.31055000	-2.59454700	1.58774900
H	3.54820000	-1.24376500	2.73095400
H	1.92547400	-1.70867600	2.22880300
C	5.34647900	0.34892400	1.26926300
H	5.45764800	-0.20787200	2.20412000
H	6.35206300	0.53110900	0.87564500
H	4.90605600	1.32072200	1.51517000
C	-5.49028900	-1.87374800	-1.31598400
H	-5.33513800	-1.74214300	-2.39123300
H	-5.93256000	-2.86470900	-1.16919000
H	-6.22538800	-1.13058000	-0.99155700



Ni	-0.10104400	1.84628300	0.23126300
C	-1.34610900	2.49031900	-0.87602500
C	-0.52662300	1.92611000	1.97277400
C	1.34498800	2.88311500	0.03260300
O	-2.09772000	2.96500200	-1.60431700
O	2.18303000	3.66522800	-0.03697400
O	-0.73536900	2.03872100	3.09385300
C	-0.25960600	-2.31138300	-0.47734500
C	1.02077400	-2.09574400	-0.85264200
H	-0.86725700	-3.19671600	-0.40105500
H	1.78878700	-2.72863100	-1.26159600
C	0.15965000	-0.10553300	-0.21019100
N	-0.77034600	-1.09045100	-0.08231500
N	1.26463300	-0.74565600	-0.68596500
C	-2.17314100	-0.88793000	0.30126000
H	-2.20161300	0.07458300	0.80552200
C	2.55844700	-0.08375000	-0.91853600
H	2.30828900	0.91858200	-1.25907700
C	-2.73534300	-1.97170100	1.28914300
C	3.49012400	-0.68847300	-2.03414200
O	-2.63214100	-3.16198300	0.92116400
O	-3.29833600	-1.50709000	2.29889400
O	3.40414700	-1.90503000	-2.30160100
O	4.28481300	0.15677900	-2.48837400
C	-3.03765800	-0.85581200	-0.96482400
H	-2.68617200	-0.04256800	-1.61285800
C	3.37452200	0.06153600	0.37497500

H	4.22279700	0.69356000	0.09779600
C	3.89302400	-1.23992800	1.01297100
H	4.01585800	-1.97841300	0.21281300
C	-4.54151700	-0.70487500	-0.72013400
H	-4.85962600	-1.55992000	-0.11308300
C	-5.29223100	-0.75801600	-2.04973200
H	-5.07227800	-1.68224100	-2.59280700
H	-6.37589400	-0.70610100	-1.89610100
H	-5.00649200	0.08219400	-2.69292600
C	5.26448600	-1.00889900	1.64762300
H	5.20888500	-0.23524100	2.42327700
H	5.64464800	-1.92281000	2.11825800
H	5.99196600	-0.68250700	0.89951400
C	-4.88807400	0.56673600	0.05097500
H	-4.51984200	1.45635000	-0.47151100
H	-5.97388500	0.66738700	0.16230200
H	-4.45175400	0.53727300	1.05090200
C	2.92478300	-1.80421000	2.05186600
H	3.30049200	-2.74557600	2.46860500
H	2.79775600	-1.09919000	2.88165500
H	1.93866100	-1.99883100	1.62870600
H	2.78119400	0.61798300	1.11079600
H	-2.86566600	-1.79470700	-1.50141500



Ni	0.03340800	1.99969900	0.01102500
C	1.58566800	2.77462700	-0.41998700
C	-1.20081700	2.53618000	-1.17142200
C	-0.32833000	2.42879200	1.70968500
O	2.52478400	3.38711200	-0.67210900
O	-1.95710400	2.90469100	-1.95089400
O	-0.52553700	2.72051500	2.80193800
N	1.01791900	-0.88065900	-0.37804300
N	-1.01474100	-0.82031600	0.28664600
C	0.02599900	-0.01414500	-0.04864700
C	-0.67808400	-2.15519700	0.17543600
H	-1.40810900	-2.91555800	0.40869000
C	0.60723100	-2.19317500	-0.24440600
H	1.29704800	-2.99561400	-0.45793600
C	2.35358300	-0.52838400	-0.84900100
H	2.31593000	0.53475600	-1.07707700
C	-2.33542500	-0.37552400	0.72392300
H	-2.25557700	0.70338000	0.84992700
C	3.47430900	-0.85284400	0.12972300
H	4.31359100	-0.17517300	-0.06249200
C	-3.46839500	-0.73705900	-0.22868700
H	-3.14580100	-0.63642700	-1.26893600
H	3.15956700	-0.65546300	1.15824600
H	-4.27960800	-0.01255700	-0.09659900
H	2.53268100	-1.08636400	-1.77104100
H	-2.53771400	-0.83805600	1.69296800
C	4.05729300	-2.29886700	0.05341900
C	-4.11111700	-2.14677800	-0.04105100
O	3.58227200	-3.05031200	-0.82915600
O	4.96102100	-2.53542900	0.87943600
O	-3.65230700	-2.85545900	0.88408800
O	-5.03827800	-2.40029600	-0.83562500



Ni	0.05812600	2.23990600	0.09986300
C	-1.52568700	3.05525300	-0.09867600
C	0.72861600	2.65680700	1.71222600
C	1.08336100	2.78957400	-1.26538500

O	1.12788000	2.94548200	2.74481400
O	1.69558400	3.17711300	-2.15199700
O	-2.48023900	3.67452000	-0.23275700
N	1.01961500	-0.60811200	-0.09323200
N	-1.11541400	-0.57601500	0.01397900
C	-0.03215400	0.24401100	0.02255300
C	-0.74616800	-1.90043700	-0.12194600
H	-1.46218100	-2.70060700	-0.08713200
C	0.60052300	-1.91987400	-0.18846300
H	1.29212300	-2.74147900	-0.22613800
C	2.40090200	-0.18963500	-0.21578100
H	2.48268800	0.79283300	0.25009200
C	-2.48857200	-0.10542300	0.02969800
H	-2.77824900	0.21060700	-0.97537700
C	3.39086400	-1.13509800	0.47671800
C	-3.48495700	-1.12954400	0.58279900
H	2.65883500	-0.07634200	-1.27251700
H	-2.52510400	0.77040600	0.67761600
O	-3.19573100	-1.85532200	1.52703800
O	3.07297200	-1.78195100	1.46642300
N	-4.67157400	-1.09842000	-0.02523000
N	4.60156900	-1.12974300	-0.08403400
H	-4.88927800	-0.51953100	-0.83872600
H	4.83909400	-0.62241300	-0.93878500
C	5.76129200	-1.84810300	0.39137800
H	6.05014800	-1.51539300	1.39202800
H	5.56087400	-2.92087800	0.45256100
C	-5.83299400	-1.87452200	0.34303700
H	-5.61589300	-2.94531900	0.31123000
H	-6.15771000	-1.64052800	1.36045800
C	-6.98575900	-1.55071400	-0.65619800
C	6.94157600	-1.59828900	-0.59681100
O	-6.69671300	-0.71808100	-1.54800500
O	8.00363400	-2.16619800	-0.29935800
O	6.67148600	-0.85436700	-1.56954300
O	-8.04728500	-2.15703600	-0.44571000

**Table S13.** Coordinates of the optimized structures.

**Precursors compounds**

**1f**

N	0.44617500	-0.02918500	0.63505700
N	-1.23506300	-0.68701700	-0.56487100
C	-0.14841900	-1.09742800	0.08593800
C	-1.36874500	0.69020300	-0.42249500
H	-2.26592600	1.23047000	-0.76030300
C	-0.30664400	1.09569200	0.32025000
H	-0.04125100	2.07643700	0.67675200
C	1.67447000	-0.04610800	1.41555000
H	1.53852400	-0.68540600	2.29220900
C	-2.24123400	-1.57837600	-1.16777800
H	-1.82352300	-2.58310400	-1.20129600
C	2.86242800	-0.59010400	0.59859400
C	-3.47642600	-1.54536500	-0.23121300
H	0.20720900	-2.10970700	0.14474100
H	1.84696800	0.96829600	1.77477700
H	-2.44011600	-1.23190100	-2.18176100
O	-3.40635300	-2.12175900	0.84246700
O	2.69578500	-1.42329600	-0.27057100
N	-4.47356300	-0.77041000	-0.69576500
N	4.07278700	-0.12123000	0.99651800
H	-4.21669600	-0.17261000	-1.47993000
H	4.11313100	0.66997700	1.61995000
C	5.29923000	-0.51467700	0.33058300
H	6.03223200	-0.88546600	1.05249300
H	5.06438700	-1.33933100	-0.34206500
C	-5.31197600	0.04134800	0.19197900
H	-6.36809800	-0.06757200	-0.06398500
H	-5.17446900	-0.28485800	1.22171000
C	-4.87519700	1.55236600	0.02457100
C	5.97687900	0.57716700	-0.48575800
O	-4.02177500	1.75018300	-0.90351400
O	6.97271500	0.39687500	-1.12855800
O	5.34970700	1.77002500	-0.38284600
H	5.84395300	2.40567600	-0.92400900
O	-5.40193900	2.34743300	0.79462300

**1g**

N	-0.75379000	0.00655600	0.28463000
N	1.24975300	0.37504300	-0.48265900
C	0.08276500	0.94261800	-0.18854800
C	1.17677000	-0.97594300	-0.19059900
H	2.08199800	-1.56879300	-0.32310600
C	-0.07835100	-1.20407400	0.28662800
H	-0.53960500	-2.11085800	0.63996600
C	-2.14455700	0.22940200	0.69029800
H	-2.28492500	1.29834800	0.84520900
C	2.45104000	1.08871300	-1.00229400
H	2.09720000	2.07808900	-1.30614200
C	-3.13683600	-0.29821400	-0.34693300
H	-2.94901000	0.14673800	-1.32933100
C	3.58506400	1.13340000	0.01275200
H	3.24927600	1.53310400	0.97493400
H	-3.04265800	-1.37867000	-0.48446100
H	4.34174500	1.83068300	-0.36271100
H	-0.15479900	1.98701700	-0.30324000

H	-2.29856400	-0.24946900	1.65771800
H	2.78104800	0.53030900	-1.87696000
C	-4.55991700	0.02151700	0.05845300
C	4.28716100	-0.26732000	0.23446900
O	-4.87323700	0.69108800	1.00896200
O	-5.44446200	-0.53440100	-0.78931400
O	3.91741400	-1.17034700	-0.57309500
O	5.10066300	-0.29841400	1.15601600
H	-6.33529700	-0.29167500	-0.49158500

## Carbene ligands

### NHC<sup>GlyGly</sup>

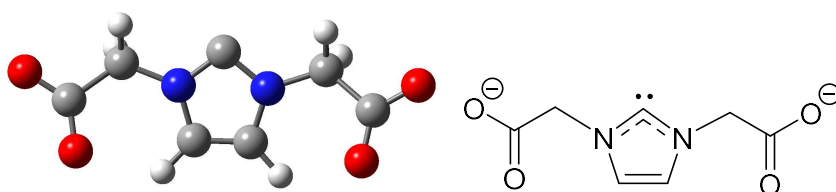
N	1.02061100	0.42888300	0.30441500
N	-1.02034300	0.42836600	-0.30372800
C	0.00009800	-0.43212400	0.00119500
C	-0.64664800	1.76707400	-0.19958300
H	-1.34684700	2.56605500	-0.36558500
C	0.64704600	1.76742100	0.19754200
H	1.34723200	2.56668700	0.36223400
C	2.30340900	-0.04593900	0.80208100
H	2.28649000	-1.12938600	0.69223500
C	-2.30308000	-0.04725600	-0.80071400
H	-2.28610300	-1.13054500	-0.68929000
C	3.53853100	0.58009800	0.12442700
C	-3.53825900	0.57953900	-0.12383500
H	2.38264300	0.17688000	1.87461600
H	-2.38227700	0.17399100	-1.87357100
O	-3.55476800	1.76297200	0.21490200
O	3.55543700	1.76361100	-0.21403000
N	-4.58056800	-0.25712800	-0.02198700
N	4.58026200	-0.25714000	0.02146300
H	-4.56818400	-1.21607700	-0.37009900
H	4.56777700	-1.21586500	0.37016800
C	5.93237600	0.10945200	-0.36763500
H	5.98726700	0.33637100	-1.43790800
H	6.25648100	1.01071400	0.16226300
C	-5.93266500	0.10988900	0.36669600
H	-5.98771200	0.33731000	1.43686800
H	-6.25656600	1.01099700	-0.16359400
C	-6.90883800	-1.08272800	0.03871400
C	6.90841300	-1.08316800	-0.03918200
O	-6.36059900	-2.09893900	-0.45869000
O	8.10055800	-0.86610800	-0.31759800
O	6.36011400	-2.09894300	0.45902700
O	-8.10102100	-0.86528600	0.31667500

### NHC<sup>β-Me</sup>

N	1.04640800	-0.23627100	0.03574500
N	-1.04493200	0.21625900	0.07539300
C	0.00136000	0.06764700	-0.79853300
C	-0.66319100	0.01315200	1.39349400
H	-1.35470000	0.08420600	2.21915100
C	0.66276400	-0.27398700	1.36832000
H	1.35315700	-0.49414300	2.16822700
C	2.42199200	-0.50416700	-0.41606500
H	2.36124300	-0.59784800	-1.50075500
C	-2.41932700	0.56412900	-0.32281300
H	-2.35907400	0.83437700	-1.37745200
C	3.45463500	0.54785800	-0.01488300
H	3.30344500	1.48084100	-0.56618000

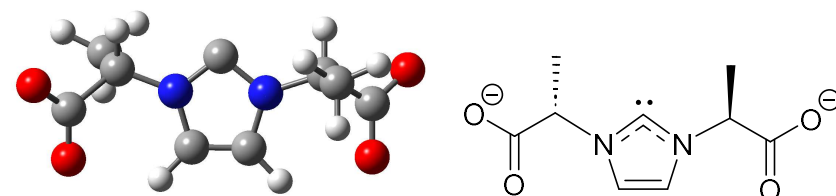
C	-3.45823700	-0.53322900	-0.09824100
H	-3.33721200	-0.95059100	0.91183900
H	3.32772800	0.79726900	1.04854200
H	-3.30859000	-1.36679200	-0.79115300
H	2.75562400	-1.46700600	-0.02308200
H	-2.74560400	1.45173900	0.22348200
C	4.95071600	0.07229200	-0.19452600
C	-4.95165900	-0.02833700	-0.20420800
O	5.78337200	0.99493100	-0.33025700
O	5.13895200	-1.16789100	-0.14480400
O	-5.13434200	1.19015200	0.03596700
O	-5.78806600	-0.91520700	-0.48163800

### NHC<sup>Gly</sup>



O	-3.43047500	1.32293100	-0.35157000
O	3.43048700	1.32293400	-0.35155200
O	4.72066500	-0.53555800	-0.34024100
N	-1.07063000	-0.35794200	0.17966300
N	1.07062900	-0.35793700	0.17967700
C	0.00000200	-1.18559700	-0.04666300
C	0.67902100	0.92311300	0.55386200
H	1.41196500	1.70081100	0.68197100
C	-0.67903000	0.92312200	0.55381000
H	-1.41197400	1.70082800	0.68187400
C	-2.45349200	-0.85256400	0.17895800
H	-2.46685000	-1.72541900	-0.47309600
C	-3.64473200	0.09744800	-0.22916500
C	2.45349200	-0.85255600	0.17897700
H	2.69679000	-1.22009000	1.18587400
C	3.64473500	0.09744900	-0.22915700
O	-4.72067200	-0.53554900	-0.34020200
H	2.46685200	-1.72542100	-0.47306400
H	-2.69679300	-1.22011400	1.18584800

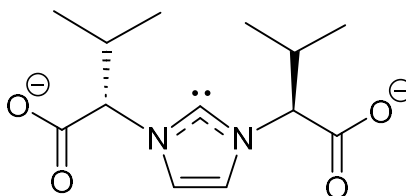
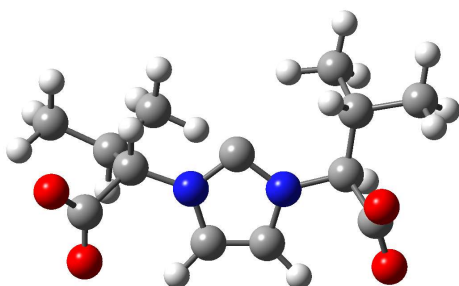
### (*S,S*)-NHC<sup>Ala</sup>



O	-3.59414600	1.40635000	-0.20795600
O	3.59419200	1.40664700	0.20558500
O	4.42681800	-0.52252700	1.04354500
N	-1.06760300	-0.17920800	0.07740300
N	1.06760600	-0.17935800	-0.07699300
C	-0.00001800	-1.03681600	0.00076100
C	0.67637300	1.15682900	-0.05614200
H	1.41556700	1.93895200	-0.09139400
C	-0.67630400	1.15693700	0.05480800

H	-1.41544300	1.93916000	0.08901800
C	-2.44565700	-0.66735000	0.27865300
H	-2.45666400	-1.66714700	-0.15232900
C	-3.59223700	0.16818100	-0.41912100
C	2.44564600	-0.66782200	-0.27762200
H	2.45671900	-1.66694800	0.15492000
C	3.59228800	0.16881500	0.41872800
O	-4.42672400	-0.52414500	-1.04290400
C	2.74968600	-0.76374900	-1.77928000
H	1.99074500	-1.36455600	-2.29180600
H	2.77007500	0.23749400	-2.21865400
H	3.73380500	-1.22241300	-1.93014700
C	-2.74987600	-0.76097700	1.78042900
H	-3.73404000	-1.21935200	1.93186500
H	-1.99104300	-1.36105600	2.29397300
H	-2.77027300	0.24093700	2.21825200

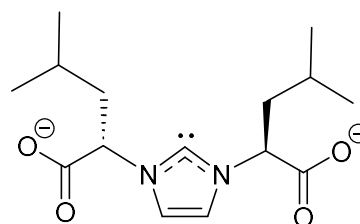
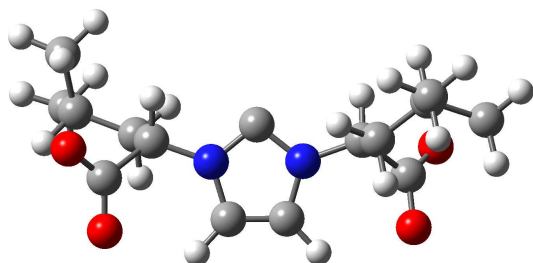
(*S,S*)-NHC<sup>Val</sup>



O	-3.47374300	-1.99112100	-0.19682900
O	3.74828500	-1.45879900	1.16223700
O	3.54492300	-2.00287800	-1.02447700
N	-1.02077400	-0.31480600	-0.02032600
N	1.09790300	-0.25490200	-0.33906400
C	0.11335500	0.32517600	0.41680100
C	0.59054600	-1.21994500	-1.20885300
H	1.25490700	-1.81611600	-1.81251200
C	-0.74952000	-1.25490200	-1.01007600
H	-1.53717700	-1.87833700	-1.39740000
C	-2.37117800	0.06054600	0.43305300
H	-2.21435800	0.61002800	1.36142600
C	-3.33127900	-1.16098200	0.73454900
C	-3.07896200	0.98364300	-0.59917400
H	-3.29155800	0.35148300	-1.47044400
C	-2.21848800	2.16896100	-1.05159300
H	-2.75644600	2.77802600	-1.79185300
H	-1.27909400	1.84040800	-1.49805600
H	-1.96150800	2.81528900	-0.20521900
C	-4.41984100	1.48545900	-0.04192700
H	-4.25717800	2.13015200	0.83071000
H	-5.05398300	0.66042000	0.28410800
H	-4.96157800	2.07327300	-0.79542200
C	2.55105500	0.05806700	-0.31730500
H	2.81507300	0.33053700	-1.34865900
C	3.37196300	-1.27905300	-0.01552000
C	2.89686700	1.25128900	0.59219500
H	2.51351500	1.01595500	1.58895400
C	2.25979700	2.56596900	0.11494100
H	2.56146600	3.40162200	0.76229300
H	1.17329700	2.49004600	0.13292400
H	2.58457900	2.80980200	-0.90642100
C	4.42173200	1.42504600	0.68788700
H	4.87361100	0.53616100	1.12481400
H	4.67048600	2.29894500	1.30510900

H	4.86398600	1.59080400	-0.30465800
O	-3.91374500	-1.11047600	1.83984000

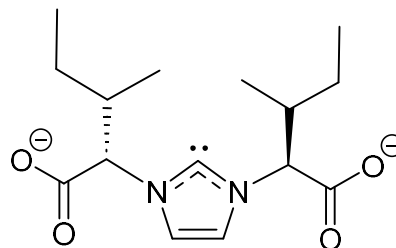
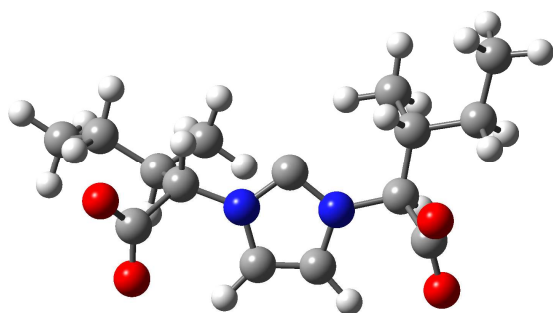
(*S,S*)-NHC<sup>Leu</sup>



O	-3.26383100	1.02174800	2.19012900
O	3.44770300	-1.57726600	1.57557400
O	3.57875900	-2.55825600	-0.45792200
N	-1.03909600	0.18184800	0.39351500
N	1.03381800	-0.33079300	0.25660700
C	-0.01620200	0.09360300	-0.51545700
C	0.67765300	-0.49206200	1.59325000
H	1.40204500	-0.82543200	2.31692500
C	-0.64008400	-0.17980800	1.67766200
H	-1.33426300	-0.12805800	2.49865600
C	-2.41446600	0.51940000	-0.01853300
H	-2.28864000	1.09140200	-0.93583200
C	-3.24834400	1.39536600	0.99380100
C	2.39839300	-0.47505800	-0.29028500
H	2.25389500	-0.68810400	-1.34955500
C	3.20837200	-1.67325800	0.34715600
O	-3.88652000	2.33316900	0.45748900
C	3.14564400	0.86584500	-0.13096600
H	2.42466200	1.66458000	-0.34303700
H	3.44195300	0.96258800	0.92074900
C	-3.18069500	-0.78492900	-0.32504800
H	-2.60540600	-1.34509000	-1.07564100
H	-3.18547300	-1.38872000	0.58996700
C	4.37283400	1.07861300	-1.04025200
H	4.04503900	0.90508500	-2.07628100
C	4.84554500	2.53788000	-0.94564000
H	5.16995900	2.77424800	0.07513500
H	5.69383100	2.73225800	-1.61469800
H	4.04440500	3.23801600	-1.20496900
C	5.53695200	0.11934800	-0.75411700
H	6.39203600	0.34022700	-1.40874800
H	5.87233200	0.21315400	0.28477700
H	5.24069400	-0.91970800	-0.90464500
C	-4.63362900	-0.61567200	-0.80646700
H	-5.19701200	-0.14423800	0.00711800
C	-4.74836200	0.30551600	-2.02802400
H	-5.77886100	0.33087500	-2.40787400
H	-4.46428400	1.32020000	-1.74540100
H	-4.09904700	-0.03382400	-2.84517200
C	-5.26011200	-1.98958400	-1.08588200
H	-5.20000700	-2.64235200	-0.20804600
H	-6.31798400	-1.90128400	-1.36537300
H	-4.74281600	-2.49956600	-1.90826100



(*S,S*)-NHC<sup>i</sup>Leu



O	-3.44662200	-2.20792400	0.15727800
O	3.78916500	-1.67824100	0.99102000
O	3.45677100	-2.37426000	-1.13594500
N	-0.99469000	-0.53906100	0.03346000
N	1.09338800	-0.52285100	-0.44798000
C	0.17623100	0.10440600	0.35324000
C	0.51115500	-1.51861500	-1.23126500
H	1.12081200	-2.15511300	-1.85116800
C	-0.81005300	-1.52654600	-0.92948100
H	-1.62936700	-2.15863800	-1.22603100
C	-2.29912600	-0.12626200	0.57633300
H	-2.05824800	0.46881400	1.45737800
C	-3.23582000	-1.32332400	1.02167700
C	-3.09755800	0.74920000	-0.43457000
H	-3.48006800	0.05286100	-1.19241300
C	-2.23774300	1.81077800	-1.13282600
H	-2.84073500	2.43348100	-1.80673200
H	-1.44211000	1.35562200	-1.72487800
H	-1.75561200	2.46677600	-0.40106300
C	-4.30824100	1.39205900	0.27670700
H	-3.95671800	2.26375100	0.84776000
H	-4.69847300	0.68827200	1.01583200
C	2.55074400	-0.24214500	-0.53725800
H	2.75569300	-0.06360600	-1.60160100
C	3.35579300	-1.57437300	-0.17673100
C	2.95937700	1.02123600	0.24758300
H	2.60217200	0.88685000	1.27333700
C	2.31209900	2.28659500	-0.33919400
H	2.56828600	3.18162200	0.24038300
H	1.22757400	2.18901800	-0.33214100
H	2.65021100	2.45336000	-1.37174100
C	4.49668300	1.15349300	0.28583200
H	4.89211100	0.21383800	0.67105700
H	4.87932700	1.27195600	-0.73995500
O	-3.73653500	-1.20456300	2.16299700
C	-5.43853200	1.82210400	-0.66515500
H	-6.27089600	2.27410200	-0.11109400
H	-5.10780100	2.55532500	-1.40989500
H	-5.83766100	0.95911900	-1.20884600
C	5.01714800	2.30633300	1.15301600
H	6.11236100	2.28419900	1.21853000
H	4.73504000	3.29308000	0.76998600
H	4.62803000	2.22896900	2.17470400

## Silver complexes



Ag	0.00000000	0.00000000	0.00022100
N	-0.96920700	2.97112200	0.46942700
N	0.96929300	2.97090500	-0.46928600
C	0.00000000	2.14120300	0.00016900
C	0.61321200	4.29982000	-0.28649800
H	1.25674000	5.09034900	-0.62502900
C	-0.61282100	4.29995900	0.28663800
H	-1.25619300	5.09063800	0.62510500
C	-2.26617900	2.51376100	0.98401300
H	-2.15051000	1.46723400	1.26302100
C	2.26610600	2.51328800	-0.98402100
H	2.15022900	1.46678100	-1.26302400
C	-2.81981800	3.35499300	2.15694900
C	2.81972000	3.35448200	-2.15698600
H	-2.99967300	2.56332300	0.17211600
H	2.99969400	2.56273600	-0.17220400
O	2.71216300	4.58214200	-2.16294500
O	-2.71230000	4.58265600	2.16289200
N	3.46852400	2.64255900	-3.07930200
N	-3.46871700	2.64309400	3.07921400
H	3.61787200	1.63081500	-3.03742500
H	-3.61806900	1.63135000	3.03734000
C	-4.25586200	3.20004200	4.17016000
H	-3.60830700	3.65733800	4.92505300
H	-4.92290800	3.98497400	3.80194000
C	4.25557700	3.19948000	-4.17032700
H	3.60795800	3.65677200	-4.92516800
H	4.92266400	3.98441000	-3.80217900
C	5.09686600	2.04101900	-4.82948300
C	-5.09722600	2.04160100	4.82925400
O	4.91178500	0.90492800	-4.32516300
O	-5.83200900	2.40564500	5.76161700
O	-4.91209800	0.90549800	4.32497700
O	5.83156700	2.40504100	-5.76191900
N	0.96920700	-2.97112200	0.46942700
N	-0.96929300	-2.97090500	-0.46928600
C	0.00000000	-2.14120300	0.00016900
C	-0.61321200	-4.29982000	-0.28649800
H	-1.25674000	-5.09034900	-0.62502900
C	0.61282100	-4.29995900	0.28663800
H	1.25619300	-5.09063800	0.62510500
C	2.26617900	-2.51376100	0.98401300
H	2.15051000	-1.46723400	1.26302100
C	-2.26610600	-2.51328800	-0.98402100
H	-2.15022900	-1.46678100	-1.26302400
C	2.81981800	-3.35499300	2.15694900
C	-2.81972000	-3.35448200	-2.15698600
H	2.99967300	-2.56332300	0.17211600
H	-2.99969400	-2.56273600	-0.17220400
O	-2.71216300	-4.58214200	-2.16294500
O	2.71230000	-4.58265600	2.16289200
N	-3.46852400	-2.64255900	-3.07930200
N	3.46871700	-2.64309400	3.07921400
H	-3.61787200	-1.63081500	-3.03742500
H	3.61806900	-1.63135000	3.03734000
C	4.25586200	-3.20004200	4.17016000
H	3.60830700	-3.65733800	4.92505300
H	4.92290800	-3.98497400	3.80194000
C	-4.25557700	-3.19948000	-4.17032700
H	-3.60795800	-3.65677200	-4.92516800
H	-4.92266400	-3.98441000	-3.80217900
C	-5.09686600	-2.04101900	-4.82948300
C	5.09722600	-2.04160100	4.82925400

O	-4.91178500	-0.90492800	-4.32516300
O	5.83200900	-2.40564500	5.76161700
O	4.91209800	-0.90549800	4.32497700
O	-5.83156700	-2.40504100	-5.76191900



Ag	0.00001400	-0.00007800	0.00001900
N	2.98257200	-0.98176100	-0.43996400
N	2.98246700	0.98179900	0.44003000
C	2.15158000	-0.00005800	0.00009800
C	4.31114700	0.62048800	0.27615000
H	5.08754100	1.30803100	0.57851600
C	4.31121400	-0.62020200	-0.27631900
H	5.08767700	-1.30761900	-0.57879900
C	2.55662100	-2.27485600	-1.00018600
H	1.46713300	-2.28117600	-0.92408800
C	2.55637700	2.27477200	1.00042200
H	1.46687600	2.28090600	0.92450700
C	3.02408400	-2.53073900	-2.43610100
H	2.32506600	-3.22954900	-2.91118300
C	3.02402500	2.53063000	2.43628200
H	2.96464500	1.60962200	3.02680200
H	2.96450600	-1.60977100	-3.02666200
H	2.32498400	3.22932600	2.91150200
H	2.96150400	-3.06037500	-0.35834400
H	2.96100600	3.06041800	0.35857400
C	4.46663000	-3.14628000	-2.60357500
C	4.46651100	3.14635400	2.60358300
O	5.14003400	-3.28389300	-1.54881300
O	4.76848100	-3.43738800	-3.77706200
O	5.13970300	3.28422300	1.54872200
O	4.76854800	3.43729100	3.77706800
N	-2.98245600	0.98173800	-0.44012500
N	-2.98253000	-0.98177900	0.43997000
C	-2.15155900	-0.00006000	-0.00009500
C	-4.31117900	-0.62028700	0.27622200
H	-5.08763800	-1.30770900	0.57869700
C	-4.31113300	0.62036000	-0.27634600
H	-5.08753200	1.30784800	-0.57882800
C	-2.55639600	2.27471800	-1.00052500
H	-1.46689500	2.28089000	-0.92460300
C	-2.55655800	-2.27480500	1.00032900
H	-1.46706500	-2.28108600	0.92429600
C	-3.02406500	2.53055000	-2.43638100
H	-2.32505400	3.22926000	-2.91162100
C	-3.02409300	-2.53058300	2.43623900
H	-2.96456700	-1.60956800	3.02673300
H	-2.96467500	1.60953600	-3.02689000
H	-2.32508100	-3.22933800	2.91141300
H	-2.96106200	3.06034900	-0.35868400
H	-2.96136700	-3.06040100	0.35853300
C	-4.46657700	3.14622300	-2.60365000
C	-4.46663100	-3.14615000	2.60368400
O	-5.13975900	3.28404300	-1.54877300
O	-4.76862700	3.43721500	-3.77711600
O	-5.13994300	-3.28393600	1.54889000
O	-4.76856500	-3.43709900	3.77719200



Ag	-0.26441100	0.06107000	-0.39706300
N	0.60971900	3.10257800	-0.79568700
N	-1.41552600	2.95369200	-0.08765300
C	-0.35441000	2.20330900	-0.46339500

C	-1.12131300	4.30075400	-0.16967000
H	-1.84406100	5.06080600	0.07653200
C	0.15619400	4.39889200	-0.61591800
H	0.76359900	5.26070800	-0.83784300
C	1.93290700	2.73776700	-1.30501300
H	2.21968200	3.46655500	-2.06481900
C	-2.72329900	2.40065100	0.31705100
H	-2.94918800	1.56736300	-0.35096300
C	2.99928700	2.62875900	-0.21182400
H	3.35692600	3.61040400	0.11378200
C	-2.78218100	1.95320900	1.78177200
H	-2.80674700	2.82247300	2.44576400
H	2.56576600	2.15797900	0.67659800
H	-1.91483200	1.33758700	2.02921800
H	1.83181300	1.78210000	-1.81265900
H	-3.47760800	3.16373100	0.12961500
C	4.19843300	1.77895400	-0.64498500
C	-4.07318500	1.11837500	1.91971900
O	4.20628900	1.29876200	-1.80159700
O	5.10415100	1.55559900	0.22331500
O	-5.15585300	1.74918300	1.79505200
O	-3.94559900	-0.12926500	2.00893500
N	-1.28516000	-2.89111200	-0.31692400
N	0.86317600	-2.92885600	-0.41051600
C	-0.20037900	-2.08323400	-0.33865000
C	0.44151900	-4.24864600	-0.43620200
H	1.12899200	-5.07681900	-0.48379900
C	-0.91350400	-4.21956300	-0.38343700
H	-1.63759500	-5.01736000	-0.38453500
C	-2.67812800	-2.41127300	-0.22060800
H	-2.69107900	-1.57847000	0.48505700
C	2.26020700	-2.50507700	-0.31391300
H	2.27336200	-1.44274300	-0.55597300
C	-3.28762300	-1.99497000	-1.56362200
H	-2.60679900	-1.33561900	-2.10587200
C	2.84248700	-2.75049800	1.08783100
H	3.12310700	-3.80279200	1.20742300
H	-3.49807000	-2.87645700	-2.17660700
H	2.08864500	-2.53759500	1.84661400
H	-3.27173400	-3.20748900	0.22684000
H	2.83939300	-3.02150900	-1.08179800
C	-4.58913300	-1.23881500	-1.22126200
C	4.06719600	-1.88449000	1.39031700
O	-4.57702400	0.01252600	-1.34118800
O	-5.51422400	-1.93017100	-0.71904100
O	4.87211300	-1.62347300	0.43568300
O	4.19421100	-1.44507000	2.55414700
Na	5.52029600	-0.39525500	-1.21349200
Na	5.37448000	0.33210000	1.99708400
Na	-5.89429300	-0.10653800	0.64034200



Ag	0.00001400	-0.00007800	0.00001900
N	2.98257200	-0.98176100	-0.43996400
N	2.98246700	0.98179900	0.44003000
C	2.15158000	-0.00005800	0.00009800
C	4.31114700	0.62048800	0.27615000
H	5.08754100	1.30803100	0.57851600
C	4.31121400	-0.62020200	-0.27631900
H	5.08767700	-1.30761900	-0.57879900
C	2.55662100	-2.27485600	-1.00018600
H	1.46713300	-2.28117600	-0.92408800
C	2.55637700	2.27477200	1.00042200
H	1.46687600	2.28090600	0.92450700
C	3.02408400	-2.53073900	-2.43610100
H	2.32506600	-3.22954900	-2.91118300
C	3.02402500	2.53063000	2.43628200

H	2.96464500	1.60962200	3.02680200
H	2.96450600	-1.60977100	-3.02666200
H	2.32498400	3.22932600	2.91150200
H	2.96150400	-3.06037500	-0.35834400
H	2.96100600	3.06041800	0.35857400
C	4.46663000	-3.14628000	-2.60357500
C	4.46651100	3.14635400	2.60358300
O	5.14003400	-3.28389300	-1.54881300
O	4.76848100	-3.43738800	-3.77706200
O	5.13970300	3.28422300	1.54872200
O	4.76854800	3.43729100	3.77706800
N	-2.98245600	0.98173800	-0.44012500
N	-2.98253000	-0.98177900	0.43997000
C	-2.15155900	-0.00006000	-0.00009500
C	-4.31117900	-0.62028700	0.27622200
H	-5.08763800	-1.30770900	0.57869700
C	-4.31113300	0.62036000	-0.27634600
H	-5.08753200	1.30784800	-0.57882800
C	-2.55639600	2.27471800	-1.00052500
H	-1.46689500	2.28089000	-0.92460300
C	-2.55655800	-2.27480500	1.00032900
H	-1.46706500	-2.28108600	0.92429600
C	-3.02406500	2.53055000	-2.43638100
H	-2.32505400	3.22926000	-2.91162100
C	-3.02409300	-2.53058300	2.43623900
H	-2.96456700	-1.60956800	3.02673300
H	-2.96467500	1.60953600	-3.02689000
H	-2.32508100	-3.22933800	2.91141300
H	-2.96106200	3.06034900	-0.35868400
H	-2.96136700	-3.06040100	0.35853300
C	-4.46657700	3.14622300	-2.60365000
C	-4.46663100	-3.14615000	2.60368400
O	-5.13975900	3.28404300	-1.54877300
O	-4.76862700	3.43721500	-3.77711600
O	-5.13994300	-3.28393600	1.54889000
O	-4.76856500	-3.43709900	3.77719200



Ag	0.00001400	-0.00007800	0.00001900
N	2.98257200	-0.98176100	-0.43996400
N	2.98246700	0.98179900	0.44003000
C	2.15158000	-0.00005800	0.00009800
C	4.31114700	0.62048800	0.27615000
H	5.08754100	1.30803100	0.57851600
C	4.31121400	-0.62020200	-0.27631900
H	5.08767700	-1.30761900	-0.57879900
C	2.55662100	-2.27485600	-1.00018600
H	1.46713300	-2.28117600	-0.92408800
C	2.55637700	2.27477200	1.00042200
H	1.46687600	2.28090600	0.92450700
C	3.02408400	-2.53073900	-2.43610100
H	2.32506600	-3.22954900	-2.91118300
C	3.02402500	2.53063000	2.43628200
H	2.96464500	1.60962200	3.02680200
H	2.96450600	-1.60977100	-3.02666200
H	2.32498400	3.22932600	2.91150200
H	2.96150400	-3.06037500	-0.35834400
H	2.96100600	3.06041800	0.35857400
C	4.46663000	-3.14628000	-2.60357500
C	4.46651100	3.14635400	2.60358300
O	5.14003400	-3.28389300	-1.54881300
O	4.76848100	-3.43738800	-3.77706200
O	5.13970300	3.28422300	1.54872200
O	4.76854800	3.43729100	3.77706800
N	-2.98245600	0.98173800	-0.44012500
N	-2.98253000	-0.98177900	0.43997000
C	-2.15155900	-0.00006000	-0.00009500

C	-4.31117900	-0.62028700	0.27622200
H	-5.08763800	-1.30770900	0.57869700
C	-4.31113300	0.62036000	-0.27634600
H	-5.08753200	1.30784800	-0.57882800
C	-2.55639600	2.27471800	-1.00052500
H	-1.46689500	2.28089000	-0.92460300
C	-2.55655800	-2.27480500	1.00032900
H	-1.46706500	-2.28108600	0.92429600
C	-3.02406500	2.53055000	-2.43638100
H	-2.32505400	3.22926000	-2.91162100
C	-3.02409300	-2.53058300	2.43623900
H	-2.96456700	-1.60956800	3.02673300
H	-2.96467500	1.60953600	-3.02689000
H	-2.32508100	-3.22933800	2.91141300
H	-2.96106200	3.06034900	-0.35868400
H	-2.96136700	-3.06040100	0.35853300
C	-4.46657700	3.14622300	-2.60365000
C	-4.46663100	-3.14615000	2.60368400
O	-5.13975900	3.28404300	-1.54877300
O	-4.76862700	3.43721500	-3.77711600
O	-5.13994300	-3.28393600	1.54889000
O	-4.76856500	-3.43709900	3.77719200



Ag	0.00000000	0.00000000	0.01860000
O	2.20820000	-3.28380000	3.25440000
O	5.08150000	2.34400000	-1.81400000
O	3.32010000	2.75470000	-3.16890000
N	2.84230000	-1.39980000	0.43420000
N	3.10870000	0.55320000	-0.45220000
C	2.14930000	-0.30680000	0.00240000
C	4.37290000	0.00230000	-0.30430000
H	5.23880000	0.55500000	-0.62530000
C	4.20480000	-1.22420000	0.24750000
H	4.89540000	-1.97910000	0.58090000
C	2.25790000	-2.66350000	0.93460000
H	1.21450000	-2.44220000	1.16190000
C	2.96130000	-3.15750000	2.26850000
C	2.84100000	1.91230000	-0.98520000
H	1.86330000	1.84740000	-1.46160000
C	3.85910000	2.36510000	-2.11240000
O	4.18720000	-3.42130000	2.16590000
O	-5.08140000	-2.34410000	-1.81400000
O	-2.20820000	3.28380000	3.25430000
O	-4.18720000	3.42140000	2.16590000
N	-3.10860000	-0.55320000	-0.45230000
N	-2.84240000	1.39980000	0.43410000
C	-2.14930000	0.30680000	0.00240000
C	-4.20480000	1.22410000	0.24750000
H	-4.89540000	1.97900000	0.58080000
C	-4.37290000	-0.00230000	-0.30430000
H	-5.23870000	-0.55500000	-0.62530000
C	-2.84100000	-1.91230000	-0.98520000
H	-1.86330000	-1.84740000	-1.46150000
C	-3.85900000	-2.36520000	-2.11240000
C	-2.25800000	2.66350000	0.93450000
H	-1.21450000	2.44230000	1.16180000
C	-2.96130000	3.15760000	2.26840000
O	-3.31990000	-2.75480000	-3.16880000
C	-2.74010000	-2.95050000	0.16850000
H	-1.89430000	-2.62690000	0.78920000
C	-2.34830000	3.77220000	-0.14550000
H	-3.41770000	3.96650000	-0.28790000
C	-1.73900000	3.35980000	-1.49180000
H	-2.23010000	2.48000000	-1.91190000
H	-1.83470000	4.17550000	-2.21810000
H	-0.67360000	3.12890000	-1.39690000

C	-1.70350000	5.06870000	0.36810000
H	-2.17680000	5.40920000	1.29120000
H	-0.63780000	4.92330000	0.57100000
H	-1.79490000	5.86120000	-0.38410000
C	-3.97880000	-3.01640000	1.07340000
H	-4.86260000	-3.29590000	0.49500000
H	-3.81640000	-3.75530000	1.86720000
H	-4.17760000	-2.05480000	1.55230000
C	-2.40770000	-4.34040000	-0.39440000
H	-1.53670000	-4.31050000	-1.05330000
H	-2.19520000	-5.03850000	0.42260000
H	-3.24500000	-4.73270000	-0.97890000
C	2.74020000	2.95050000	0.16850000
H	1.89440000	2.62690000	0.78910000
C	3.97890000	3.01640000	1.07330000
H	4.86270000	3.29590000	0.49490000
H	3.81660000	3.75530000	1.86710000
H	4.17770000	2.05480000	1.55230000
C	2.40780000	4.34040000	-0.39450000
H	1.53680000	4.31040000	-1.05340000
H	2.19520000	5.03850000	0.42250000
H	3.24510000	4.73270000	-0.97900000
C	2.34810000	-3.77220000	-0.14530000
H	3.41760000	-3.96650000	-0.28780000
C	1.73880000	-3.35980000	-1.49160000
H	2.23000000	-2.48000000	-1.91180000
H	1.83450000	-4.17550000	-2.21800000
H	0.67340000	-3.12890000	-1.39680000
C	1.70340000	-5.06870000	0.36830000
H	2.17670000	-5.40920000	1.29130000
H	0.63760000	-4.92320000	0.57120000
H	1.79470000	-5.86120000	-0.38390000



Ag	0.00530000	0.03910000	0.09040000
O	-3.18560000	-3.04690000	2.36820000
O	4.16080000	-4.04880000	-0.69610000
O	4.40750000	-2.21330000	-1.99030000
N	-0.55830000	-3.08640000	0.19040000
N	1.56250000	-2.74280000	-0.04540000
C	0.36830000	-2.09300000	0.07310000
C	1.38010000	-4.11690000	0.00200000
H	2.22780000	-4.77390000	-0.08610000
C	0.04900000	-4.33180000	0.14580000
H	-0.53680000	-5.22450000	0.27840000
C	-2.02410000	-2.90560000	0.27040000
H	-2.18260000	-1.84510000	0.46770000
C	-2.63500000	-3.72920000	1.47990000
C	2.87840000	-2.06160000	-0.16270000
H	2.67190000	-1.13510000	-0.69780000
C	3.90950000	-2.86790000	-1.04900000
O	-2.53240000	-4.97870000	1.38650000
O	-4.24980000	3.97640000	-0.82830000
O	2.96040000	3.36980000	2.55050000
O	2.35550000	5.22030000	1.39690000
N	-1.60110000	2.76800000	-0.11780000
N	0.49240000	3.19170000	0.21570000
C	-0.39160000	2.16370000	0.06700000
C	-0.15650000	4.41340000	0.11990000
H	0.39210000	5.32810000	0.26320000
C	-1.47040000	4.14780000	-0.08400000
H	-2.33760000	4.77160000	-0.21640000
C	-2.88660000	2.04270000	-0.28880000
H	-2.63150000	1.12950000	-0.82550000
C	-3.91710000	2.82280000	-1.20600000
C	1.95730000	3.06910000	0.38560000

H	2.14200000	2.02770000	0.65090000
C	2.46850000	3.98080000	1.58150000
O	-4.32250000	2.17800000	-2.19560000
C	-3.48370000	1.62830000	1.08680000
H	-2.75190000	0.94160000	1.53430000
C	2.70280000	3.43020000	-0.92690000
H	2.45310000	4.47800000	-1.13550000
C	2.25730000	2.56870000	-2.12390000
H	1.16590000	2.51920000	-2.14730000
H	2.60750000	1.53930000	-1.98200000
C	4.22160000	3.34550000	-0.70370000
H	4.53170000	3.99400000	0.11740000
H	4.52390000	2.32190000	-0.45960000
H	4.76880000	3.64990000	-1.60170000
C	-3.67580000	2.80350000	2.05720000
H	-4.35400000	3.54470000	1.62730000
H	-4.08310000	2.44810000	3.00920000
H	-2.72620000	3.29920000	2.27390000
C	-4.79270000	0.83930000	0.87460000
H	-4.67310000	0.18320000	0.00660000
H	-5.58530000	1.54570000	0.60120000
C	3.41110000	-1.67400000	1.24710000
H	2.61280000	-1.05720000	1.68010000
C	3.61950000	-2.86430000	2.19550000
H	4.32200000	-3.58800000	1.77850000
H	3.99740000	-2.50720000	3.16130000
H	2.67700000	-3.38500000	2.38130000
C	4.65140000	-0.74880000	1.17630000
H	4.47900000	0.00360000	0.40010000
H	4.69550000	-0.19400000	2.12110000
C	-2.70610000	-3.30970000	-1.06420000
H	-2.47620000	-4.37250000	-1.21080000
C	-2.16480000	-2.51710000	-2.26950000
H	-1.07250000	-2.50930000	-2.23540000
H	-2.48220000	-1.47070000	-2.18760000
C	-4.23200000	-3.17430000	-0.93810000
H	-4.60770000	-3.75710000	-0.09540000
H	-4.52100000	-2.12970000	-0.78480000
C	6.01490000	-1.41020000	0.92730000
H	6.04950000	-1.91970000	-0.03650000
H	6.80050000	-0.64490000	0.93430000
H	6.25810000	-2.13840000	1.70820000
C	2.74370000	3.08300000	-3.48560000
H	2.35040000	2.46190000	-4.29700000
H	2.40490000	4.11140000	-3.65830000
H	3.83490000	3.07170000	-3.56620000
C	-5.22100000	-0.00870000	2.07950000
H	-5.36330000	0.60260000	2.97790000
H	-6.17390000	-0.51100000	1.87500000
H	-4.48730000	-0.78870000	2.30570000
C	-2.59920000	-3.06930000	-3.63380000
H	-2.30300000	-4.11950000	-3.74340000
H	-3.68220000	-3.00950000	-3.77800000
H	-2.13060000	-2.50470000	-4.44650000
H	-4.73250000	-3.52830000	-1.84500000



Ag	-0.03520000	0.03180000	0.10020000
O	0.49900000	-3.89370000	-3.34620000
O	-4.34800000	-2.35730000	2.89790000
O	-4.50380000	-0.12640000	3.22070000
N	-0.93700000	-2.98940000	-0.34710000
N	-2.45440000	-1.92270000	0.76460000
C	-1.24420000	-1.76100000	0.15390000
C	-2.88750000	-3.23430000	0.64630000
H	-3.79350000	-3.55250000	1.12750000
C	-1.93330000	-3.90540000	-0.04530000



H	-1.84870000	-4.92330000	-0.38400000
C	0.33840000	-3.34550000	-1.01750000
H	0.73600000	-2.40850000	-1.40800000
C	0.10780000	-4.32300000	-2.24020000
C	-3.23930000	-0.81100000	1.35430000
H	-2.49540000	-0.09300000	1.70250000
C	-4.11150000	-1.15640000	2.63130000
O	-0.39280000	-5.44060000	-1.95820000
O	4.35210000	2.16030000	2.92170000
O	-0.46150000	4.15360000	-3.28280000
O	0.59630000	5.56650000	-1.86810000
N	2.43220000	1.88030000	0.78640000
N	0.97570000	3.04780000	-0.30560000
C	1.21760000	1.79410000	0.16870000
C	2.01660000	3.90460000	0.02120000
H	1.98710000	4.93180000	-0.29860000
C	2.93210000	3.17020000	0.69990000
H	3.85270000	3.42980000	1.18860000
C	3.16140000	0.71400000	1.34230000
H	2.38330000	0.02900000	1.68250000
C	4.06150000	0.98000000	2.61870000
C	-0.26360000	3.48480000	-0.99330000
H	-0.69450000	2.58160000	-1.42190000
C	0.00640000	4.50070000	-2.17820000
O	4.41300000	-0.08470000	3.17080000
C	3.94030000	-0.02270000	0.22660000
H	3.20590000	-0.35400000	-0.51650000
C	-1.22010000	4.10760000	0.04420000
H	-0.66220000	4.88310000	0.57940000
C	-2.49860000	4.74420000	-0.53160000
H	-2.18350000	5.53230000	-1.22480000
C	5.05180000	0.74870000	-0.51710000
H	4.65580000	1.73280000	-0.79500000
C	-4.06940000	-0.09220000	0.26450000
H	-3.36240000	0.28880000	-0.48120000
C	-5.15410000	-0.90170000	-0.47870000
H	-4.71900000	-1.86470000	-0.77130000
C	1.30330000	-3.93120000	0.03400000
H	0.92240000	-4.91310000	0.33910000
C	2.78160000	-4.05810000	-0.39140000
H	3.07070000	-3.11610000	-0.87510000
H	1.25840000	-3.27920000	0.91410000
H	4.36390000	-0.92060000	0.68680000
H	-1.49150000	3.33790000	0.77890000
H	-4.52860000	0.77520000	0.74940000
C	3.66520000	-4.22830000	0.85540000
H	3.39310000	-5.14210000	1.39930000
H	4.72300000	-4.30910000	0.57990000
H	3.56420000	-3.38550000	1.54450000
C	3.04530000	-5.19740000	-1.38830000
H	2.74720000	-6.16110000	-0.95890000
H	2.49310000	-5.06180000	-2.31870000
H	4.11530000	-5.24940000	-1.62740000
C	-5.55180000	-0.16920000	-1.77090000
H	-6.31020000	-0.73390000	-2.32640000
H	-5.97020000	0.81930000	-1.54540000
H	-4.69060000	-0.02190000	-2.42890000
C	-6.40150000	-1.18240000	0.37460000
H	-6.16290000	-1.74810000	1.27630000
H	-6.87280000	-0.24320000	0.68720000
H	-7.13850000	-1.75290000	-0.20590000
C	-3.30800000	5.40120000	0.59770000
H	-2.70730000	6.14230000	1.13650000
H	-4.19600000	5.90910000	0.20210000
H	-3.64790000	4.65440000	1.32430000
C	-3.36300000	3.74590000	-1.31380000
H	-2.82490000	3.36490000	-2.18390000
H	-3.65800000	2.90040000	-0.68340000
H	-4.28010000	4.22830000	-1.67360000
C	6.31770000	0.96660000	0.32730000
H	6.11170000	1.53150000	1.23760000

H	6.75170000	0.00520000	0.62540000
H	7.07260000	1.51220000	-0.25390000
C	5.40530000	0.01470000	-1.82140000
H	6.18210000	0.55260000	-2.37810000
H	5.78310000	-0.99340000	-1.61130000
H	4.53240000	-0.08770000	-2.47250000