Electronic Supplementary Material (ESI) for CrystEngComm.

The role of non-covalent intermolecular interactions on the diversity of crystal packing in the supramolecular dihalopyridine-silver(I) nitrate complexes

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SUPPORTING INFORMATION

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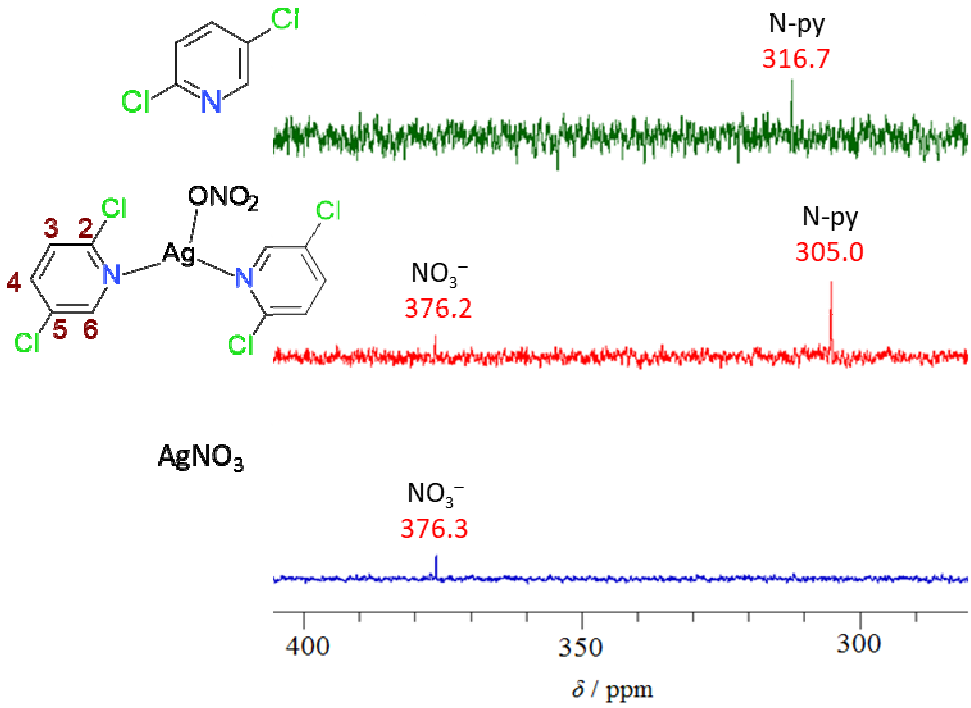
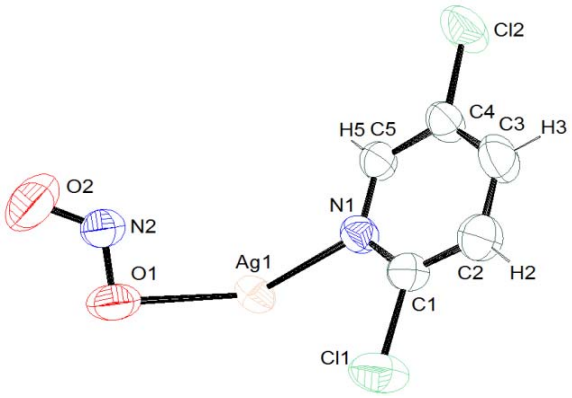
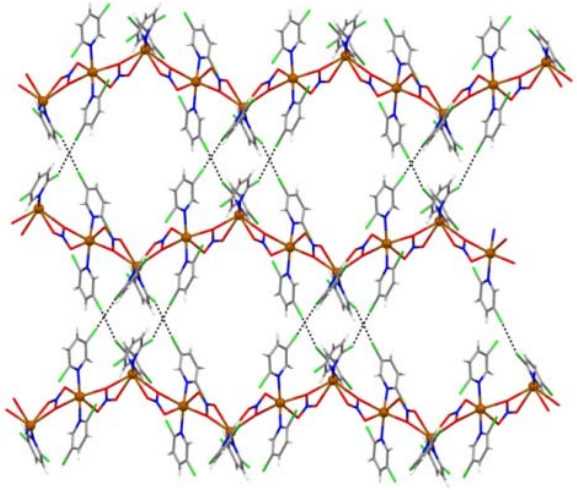


Figure S1. The chemical shift of ^{15}N pyridine and NO_3^- signals in 2,5-dichloropyridine, its silver complex (**1**) and silver(I) nitrate, recorded in dimethylformamide-d_7 at 61.8 MHz. The numbering scheme was used for the assignment of the NMR spectra.



a



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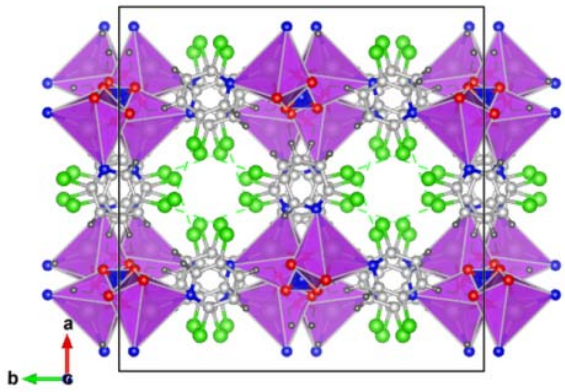
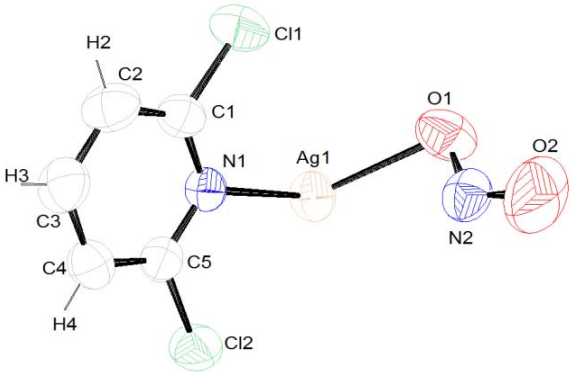
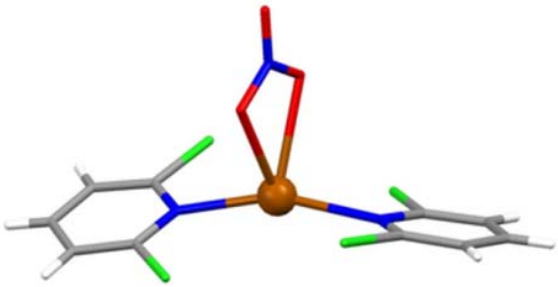


c

Figure S2. The asymmetric unit of **1** showing the atomic labels. Displacement ellipsoids are drawn at the 50% probability level (a). The linkage of neighbouring Ag–nitrate chains and 2,5-dichloropyridine ligands by the C−Cl···Cl−C halogen···halogen interactions (b); The Ag-nitrate chains (violet polyhedra of the AgN_2O_4 and blue triangle of NO_3) in channels along [001] (c).



a



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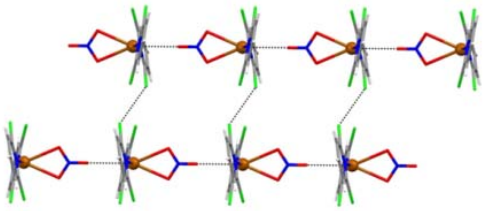

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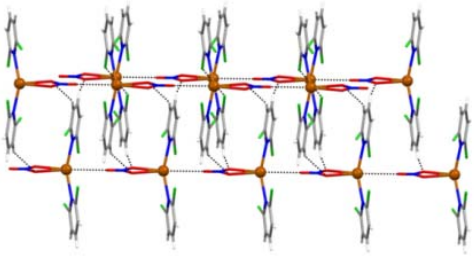

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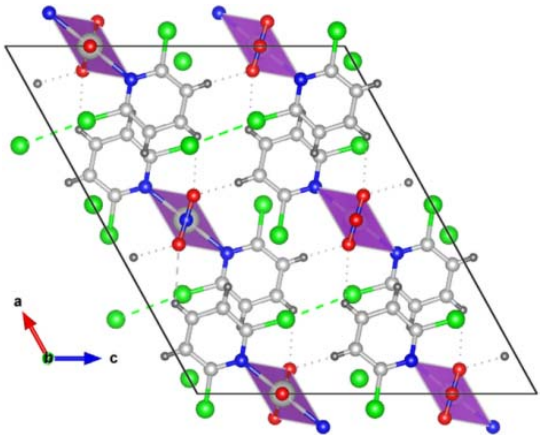


e

Figure S3. The asymmetric unit of **2** showing the atomic labels. Displacement ellipsoids are drawn at the 50% probability level (a). The distorted $Ag1N_2O_2$-tetrahedron in **2** sharing two O atoms with nitrate and two N atoms with two 2,6-Cl_2py ligands (b). The *anti*-parallel orientation of adjacent $[Ag(NO_3)(2,6\text{-}Cl_2py)_2]_n$ chains linked by the C−Cl···Cl−C halogen···halogen interactions (c). The 3D supramolecular framework formed by hydrogen bonds and intermolecular interactions (d). The view of structure down the *b*-axis showing the C–Cl···Cl–C halogen···halogen interactions and hydrogen bonds which link the 1D Ag–nitrate chains (violet polyhedra) and 2,6-dichloropyridine ligands to build the 3D structure (e).

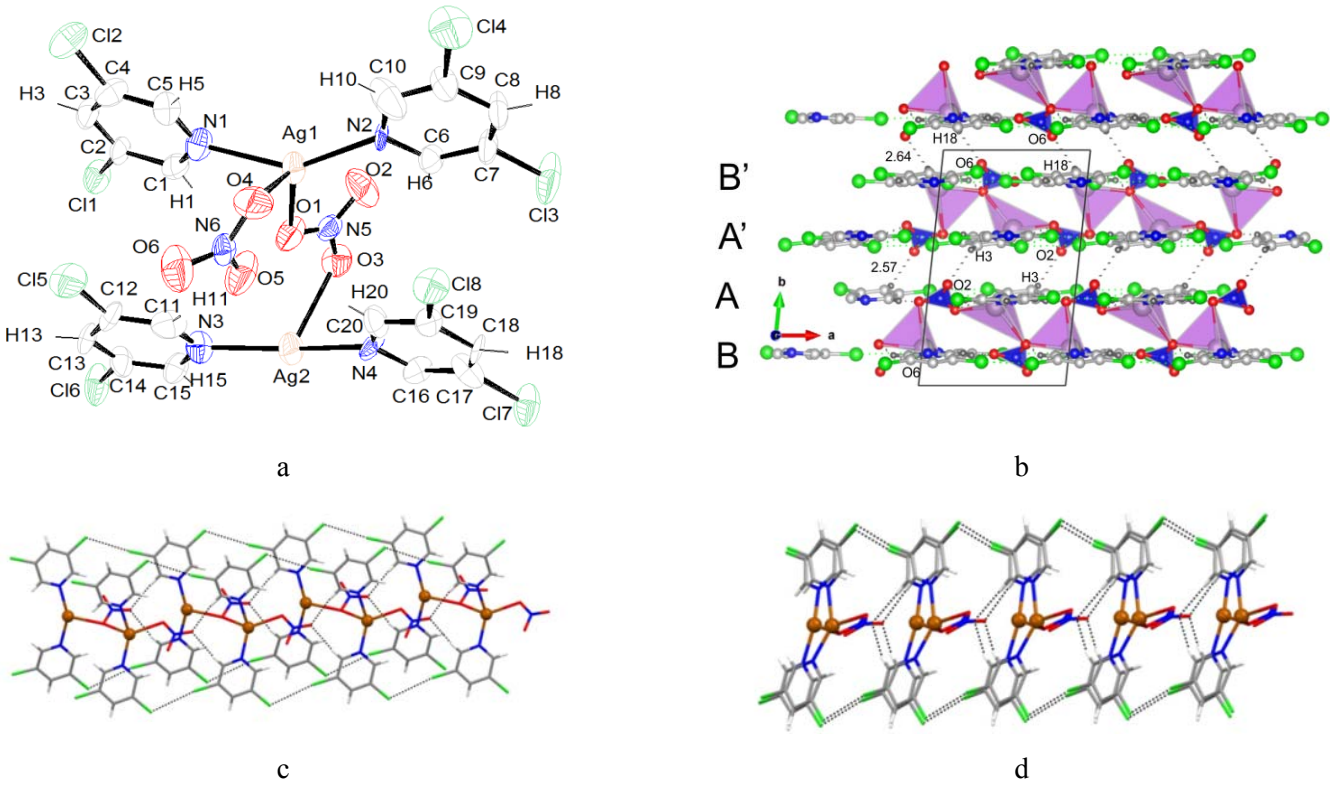
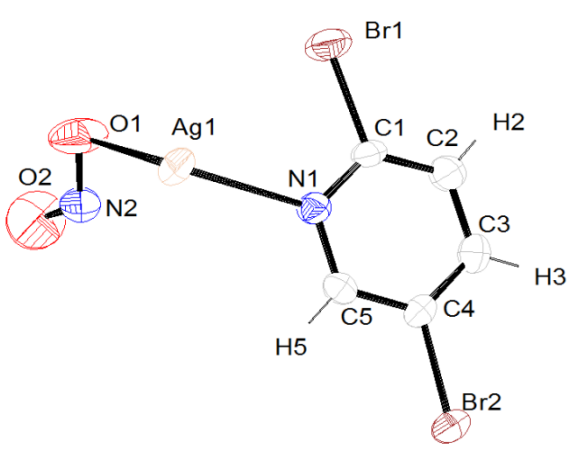


Figure S4. The asymmetric unit of **3** containing one dimer and showing the atomic labels. Displacement ellipsoids are drawn at the 50% probability level (a). The layers in **3** having a stacking sequence of B–A–A'–B' type (A–A' situated at $y \approx \pm 0.375$, B'–B situated at $y \approx \pm 0.125$) are connected by the infinite Ag-nitrate chains (violet polyhedra of the AgN_2O_2 and blue triangle of NO_3) and by the weak hydrogen bonds (b). The intermolecular non-covalent interactions between ligands in A and B layers realized through C–Cl···Cl–C halogen···halogen interactions and C–H···O hydrogen bonds roughly along [021] (c) and [210] (d).



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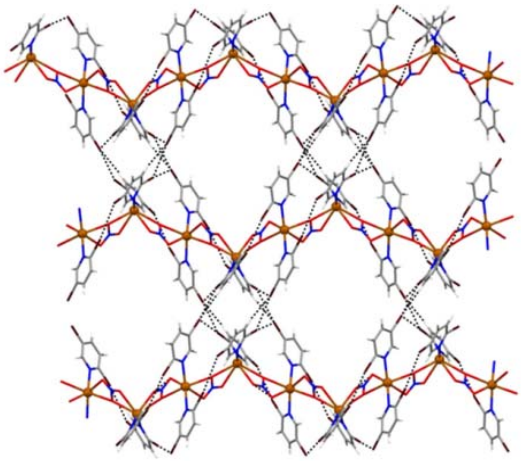

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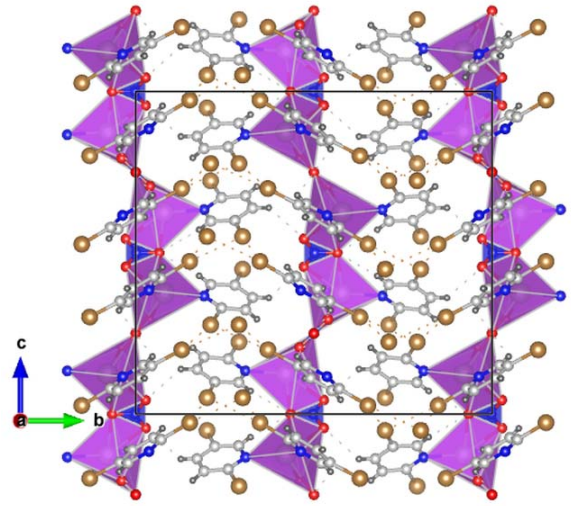
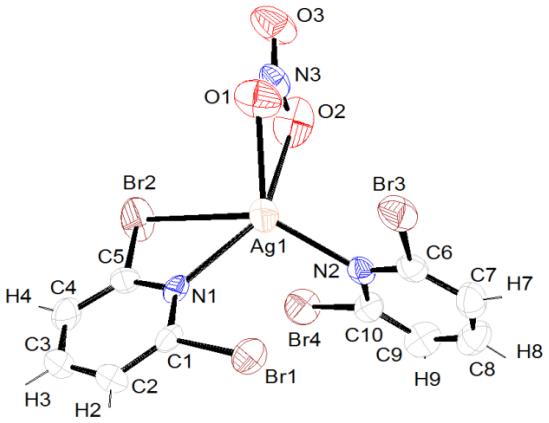


c

Figure S5. The asymmetric unit of **4** showing the atomic labels. Displacement ellipsoids are drawn at the 50% probability level (a). The C–Br···Br–C halogen···halogen interactions and C–H···O hydrogen bonds in **4** linking adjacent chains (b). The wavy polymeric Ag-nitrate chains (violet polyhedra of the AgN_2O_2 and blue triangle of NO_3) in channels along [001] (c).



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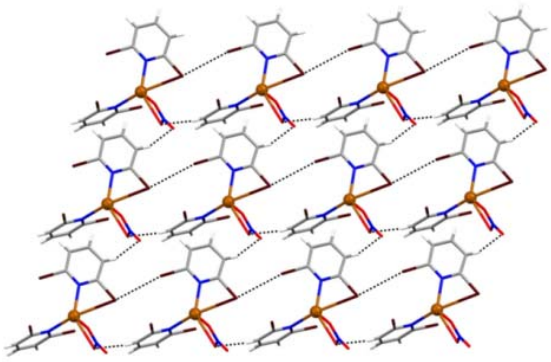

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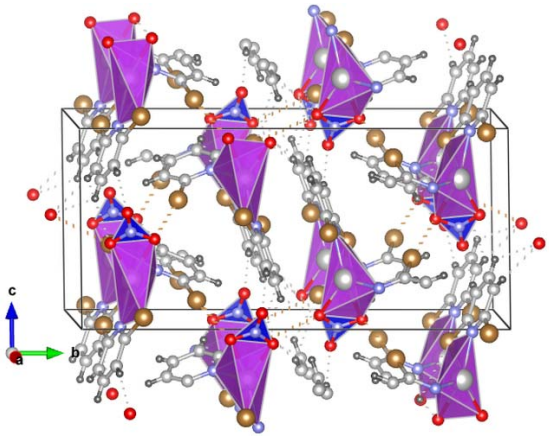

c

Figure S6. The asymmetric unit with atom labels in **5.** Displacement ellipsoids are drawn at the 50% probability level (a). 2D supramolecular layer parallel to (010) established by the interconnection of monomers *via* C–Br···Br–C halogen···halogen interactions and C–H···O hydrogen bonds (b). Polyhedral view of the structure of **5** (violet polyhedra of the AgN_2O_2Br and blue triangle of NO_3) approximately along the [100] direction showing C–H···O hydrogen bonds and C–Br···O halogen bonds (c).

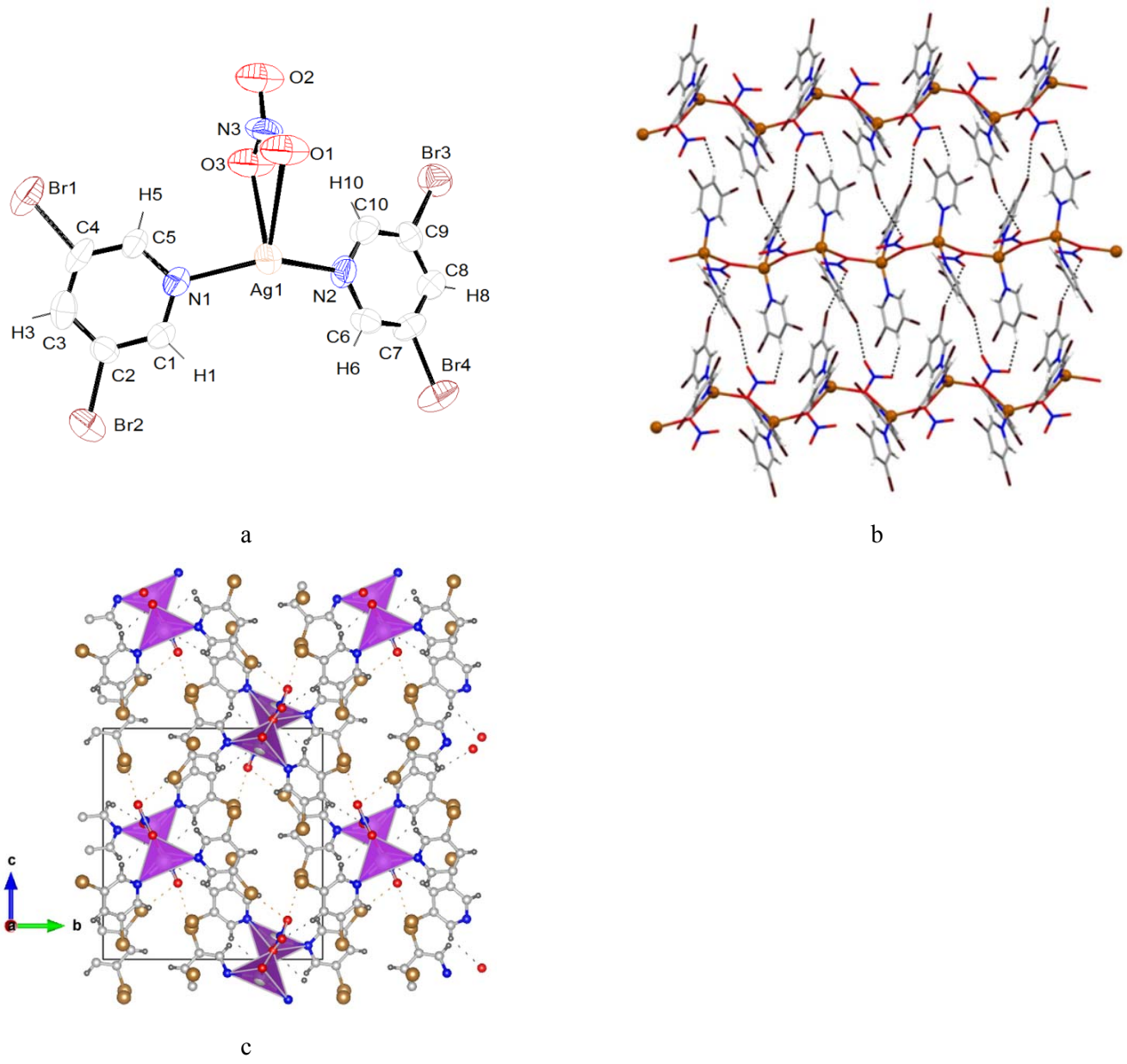

Figure S7. The asymmetric unit of **6** showing the atomic labels. Displacement ellipsoids are drawn at the 50% probability level (a). The intermolecular C–H···O hydrogen bonds and C–Br···O halogen bonds linking the chains (b). The layered structure of **6** formed by the supramolecular organizations of 3,5-Br_2py ligands with Ag-nitrate chains (violet polyhedra) between them (c).

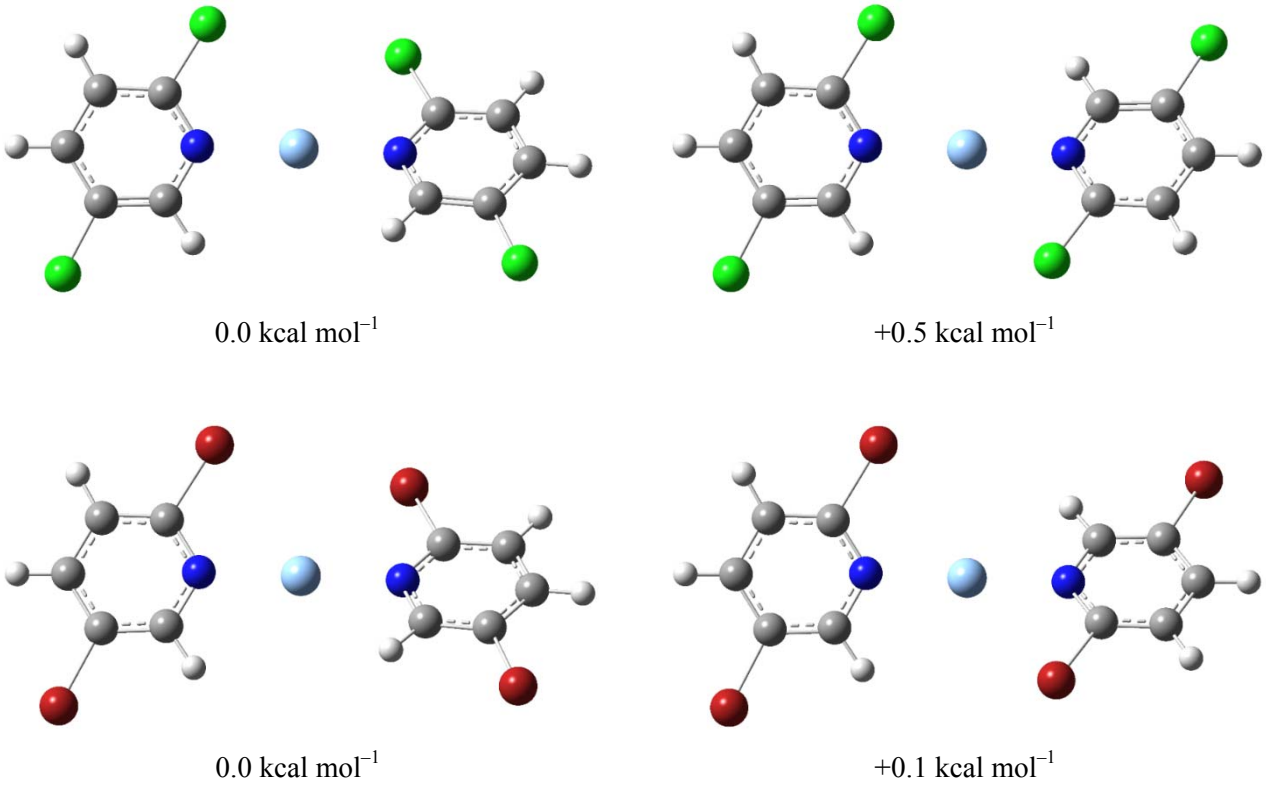

Figure S8. Relative stability of different structural isomers of 1:2 Ag^+ complexes with 2,5-Cl_2py (top, chlorine atoms in green) and 2,5-Br_2py ligands (bottom, bromine atoms in brown) calculated as a difference in the total Gibbs free energies.

Table S1a. Crystal data for compounds **1**–**3**.

	$Ag(NO_3)(2,5\text{-}Cl_2py)_2$ (1)	**$Ag(NO_3)(2,6\text{-}Cl_2py)_2$ (2)**	**$Ag(NO_3)(3,5\text{-}Cl_2py)_2$ (3)**
Crystal data			
Chemical formula	$C_{10}H_6AgCl_4N_3O_3$	$C_{10}H_6AgCl_4N_3O_3$	$C_{20}H_{12}Ag_2Cl_8N_6O_6$
M_r	465.85	465.85	931.70
Crystal system, space group	Tetragonal, $I4_1/acd$	Monoclinic, $C2/c$	Triclinic, $P\bar{1}$
Temperature (K)	296	296	296
a, b, c (Å)	19.2103 (3), 19.2103 (3), 16.6266 (5)	16.6683 (12), 7.2365 (4), 14.3065 (12)	8.2976 (5), 13.7115 (9), 14.1141 (9)
α, β, γ (°)	90, 90, 90	90, 119.049 (10), 90	73.313 (6), 80.742 (5), 81.585 (5)
V (Å^3)	6135.8 (3)	1508.6 (2)	1509.60 (17)
Z	16	4	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.02	2.05	2.05
Crystal size (mm)	0.14 x 0.30 x 0.53	0.18 x 0.41 x 0.60	0.10 x 0.16 x 0.54
Data collection			
Diffractometer	Oxford Diffraction Xcalubur	Oxford Diffraction Xcalubur	Oxford Diffraction Xcalubur
Absorption correction	Multi-scan	Multi-scan	Multi-scan
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13156, 1509, 1202	3071, 1553, 1187	10110, 10110, 7582
R_{int}	0.025	0.018	0.059
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617	0.628	0.617
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.064, 1.05	0.027, 0.072, 1.03	0.0352, 0.0903, 1.052
No. of reflections	1509	1553	10110
No. of parameters	97	98	381
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0340P)^2 + 3.4468P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.\ 0.0512P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.41, −0.31	0.34, −0.39	0.512, −0.636

Table S1b. Crystal data for compounds **4**–**6**.

	$Ag(NO_3)(2,5\text{-}Br_2py)_2$ (4)	**$Ag(NO_3)(2,6\text{-}Br_2py)_2$ (5)**	**$Ag(NO_3)(3,5\text{-}Br_2py)_2$ (6)**
Crystal data			
Chemical formula	$C_{10}H_6AgBr_4N_3O_3$	$C_{10}H_6AgBr_4N_3O_3$	$C_{10}H_6AgBr_4N_3O_3$
M_r	643.69	643.69	643.69
Crystal system, space group	Tetragonal, $I4_1/acd$	Monoclinic, $P2_1/c$	Orthorhombic, $P2_12_12_1$
Temperature (K)	296	296	296
a, b, c (Å)	19.3089 (8), 19.3089 (8), 17.5217 (12)	8.3416 (4), 20.5345 (12), 9.6839 (6)	8.1687 (6), 13.9793 (10), 14.6804 (8)
α, β, γ (°)	90, 90, 90	90, 103.852 (6), 90	90, 90, 90
V (Å^3)	6532.7 (7)	1610.52 (16)	1676.39 (19)
Z	16	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	11.03	11.19	10.75
Crystal size (mm)	0.40 x 0.51 x 0.60	0.23 x 0.66 x 0.92	0.17 x 0.25 x 0.54
Data collection			
Diffractometer	Oxford Diffraction Xcalubur	Oxford Diffraction Xcalubur	Oxford Diffraction Xcalubur
Absorption correction	Multi-scan	Multi-scan	Multi-scan
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26830, 1668, 1211	23213, 3152, 2648	6948, 3269, 2749
R_{int}	0.082	0.060	0.022
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617	0.617	0.617
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.063, 1.06	0.035, 0.094, 1.054	0.033, 0.072, 1.02
No. of reflections	1668	3152	3269
No. of parameters	98	191	191
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0292P)^2 + 6.3206P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 1.6891P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.0567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.60, −0.59	0.92, −0.90	0.50, −0.65
Absolute structure	–	–	
Absolute structure parameter	–	–	0.01 (9)

Table S2. Difference in chemical shift of ^{15}N-py ($\Delta\delta_{coord}$/ppm) atom signal between complex and free ligand ($\Delta\delta_{coord}$, N-py = $\delta_{coord} - \delta_{ligand}$).

Compound	**1**	**2**	**3**	**4**	**5**	**6**
$\Delta\delta_{coord}$ / ppm	–7.1	–1.9	–19.2	–5.6	–3.7	–14.0

Table S3a. The bond-length geometry (Å, °) with the coordinating ligands and intermolecular interactions in **1** and **4**.

[Ag(NO$_3$)(2,5-Cl$_2$py)$_2$] (1)			**[Ag(NO$_3$)(2,5-Br$_2$py)$_2$] (4)**		
Ag–N and Ag–O bonds		***Σv$_i$* (v.u.)**	**Ag–N and Ag–O bonds**		***Σv$_i$* (v.u.)**
Ag1–N1, Ag1–N1^{i}	2.299(2)	0.297×2	Ag1–N1, Ag1–N1^{i}	2.329(3)	0.274×2
Ag1–O1, Ag1–O1^{ii}	2.6588(4)	0.110×2	Ag1–O1, Ag1–O1^{ii}	2.6825(5)	0.103×2
Ag1–O2^{ii}, Ag1–O2^{iii}	2.689(3)	0.101×2	Ag1–O2^{ii}, Ag1–O2^{iii}	2.616(5)	0.123×2
	CN=6	1.018		CN=6	1.000
< Ag–N> < Ag–O>	<2.299> <2.674>		< Ag–N> < Ag–O>	<2.329> <2.650>	
Ag···O interactions			**Ag···O interactions**		
Ag···Cl interactions			**Ag···Br interactions**		
Ag1···Cl1, Ag1···Cl1^{i}	3.3197(8)	0.036×2	Ag1···Br1, Ag1···Br1^{i}	3.3664(7)	0.0451×2
Nitrate group bonds			**Nitrate group bonds**		
N2– O1	1.237(4)		N2–O1	1.226(7)	
N2–O2; N2–O2^{iii}	1.235(3)		N2–O2; N2–O2^{iii}	1.222(5)	
< N2–O>	<1.236>		< N2–O>	<1.224>	
2,5–dichloropyridine bonds			**2,5–dibromopyridine bonds**		
Cl1–C1	1.734(2)		Br1–C1	1.896(4)	
Cl2–C4	1.729(3)		Br2–C4	1.895(4)	
<Cl–C>	<1.732>		<Br–C>	<1.896>	
N1–C1	1.320(3)		N1–C1	1.323(5)	
N1–C5	1.337(3)		N1–C5	1.338(5)	
< N–C>	<1.329>		< N–C>	<1.331>	
C1–C2	1.380(4)		C1–C2	1.370(6)	
C2–C3	1.373(4)		C2–C3	1.378(6)	
C3–C4	1.376(4)		C3–C4	1.357(6)	
C4–C5	1.371(3)		C4–C5	1.374(6)	
<C–C>	<1.375>		<C–C>	<1.370>	
Cl···Cl interactions			**Br···Br interactions**		
Cl1···Cl2^{iv}	3.4301(11)		Br1···Br2^{iv}	3.5113(7)	
∠C1–Cl1···Cl2^{iv}	102.49(10)		∠C1–Br1···Br2^{iv}	97.6(2)	
∠Cl1^{vi}···Cl2–C4	173.70(10)		∠Br1^{vi} ···Br2–C4	175.06(14)	
Cl1··· Cl2^{v}	*3.6259(11)*		Br1···Br2^{v}	3.5360(7)	
∠C4–Cl2···Cl1^{ii}	*118.82(9)*		∠Br^{ii}···Br2 –C4	112.1(2)	
∠C1–Cl1···Cl2^{v}	*164.59(10)*		∠C1–Br1···Br2^{v}	170.48(13)	
Cl1–Cl1^{i}	*3.6285(17)*				
∠C1–Cl1···Cl1^{i}	*92.23(9)*				
∠Cl1···Cl1^{i} –C1^{i}	*92.23(9)*				
C–Cl···O halogen bonds			**C–Br···O halogen bonds**		
C–H···O bonds and interactions			**C–H···O bonds and interactions**		
H3···O2^{vii}	2.50		H3···O2^{vii}	2.57	
∠CHO	136		∠CHO	137	
H5···O1^{ii}	2.60		H5···O1^{ii}	2.66	
∠CHO	129		∠CHO	128	
C–H···Cl interactions			**C–H···Br interactions**		
H2···Cl2^{iv}	*3.02*		*H2···Br2^{iv}*	*2.99*	
∠C2–H2···Cl2^{iv}	*145*		*∠C2–H2···Br2^{iv}*	*148*	
C–Cl···π interactions Cg1: 0.2351, 0.2375, 0.1377			**C–Br···π interactions** Cg1: 0.2362, 0.2404, 0.1365		
Cl2···Cg1^{viii}	3.905(1)		*Br2···Cg1^{iii}*	*4.042 (2)*	
∠C4–Cl2…Cg1^{viii}	82.0(1)		*∠C4–Br2···Cg1^{iii}*	*81.5(1)*	
			Br1···Cg1^{ix}	*4.067 (2)*	
			∠C1–Br1···Cg^{ix}	*66.7(1)*	
π–stacking interactions			**π–stacking interactions**		
Cg1···Cg1^{ix}	3.809(1)		Cg1···Cg1^{viii}	4.032(2)	
Symmetry codes: (i) *y*−1/4, *x*+1/4, −*z*+1/4; (ii) *y*−1/4, −*x*+3/4, *z*+1/4; (iii) −*x*+1/2, *y*, −*z*; (iv) *y*−3/4, −*x*+1/4, *z*−1/4; (v) −*y*+3/4, *x*+1/4, *z*−1/4; (vi) −*y*+1/4, *x*+3/4, *z*+1/4; (vii) *y*−3/4, *x*+1/4, *z*+1/4; (viii) *x*, 1−*y*, 1/2−*z*; (ix) −*x*, 1−*y*, −*z*.			Symmetry codes: (i) *y*−1/4, *x*+1/4, −*z*+1/4; (ii) *y*−1/4, −*x*+3/4, *z*+1/4; (iii) −*x*+1/2, *y*, −*z*; (iv) *y*−3/4, −*x*+1/4, *z*−1/4; (v) −*y*+3/4, *x*+1/4, *z*−1/4; (vi) −*y*+1/4, *x*+3/4, *z*+1/4; (vii) *y*−3/4, *x*+1/4, *z*+1/4; (viii) −*x*, −*y*+1, −*z*; (ix) *y*+1/4, *x*+3/4, −*z*+3/4.		

Table S3b. The bond-length geometry (Å, °) with the coordinating ligands and intermolecular interactions in **2** and **5**.

[Ag(NO$_3$)(2,6-Cl$_2$py)$_2$] (2)			**[Ag(NO$_3$)(2,6-Br$_2$py)$_2$] (5)**			
Ag–N and Ag–O bonds		***Σν$_i$* (v.u.)**	**Ag–N and Ag–O bonds**		***Σν$_i$* (v.u.)**	
Ag1–N1, Ag1–N1^{i}	2.2576(19)	0.3322×2	Ag1–N2	2.301(4)	0.2957	
Ag1–O1, Ag1–O1^{i}	2.567(2)	0.1410×2	Ag1–N1	2.342(4)	0.2648	
	CN=4	0.9464	Ag1–O1	2.365(4)	0.2430	
			Ag1–O2	2.670(5)	0.1067	
			CN=4		0.9102	
< Ag–N> < Ag–O>	<2.258> <2.567>		< Ag–N> < Ag–O>	<2.322> <2.518>		
Ag···O interactions			**Ag···O interactions**			
Ag1···O2^{ii}	3.045(4)	0.0388				
	CN=4+1	0.9852				
Ag···Cl interactions			**Ag···Br interactions**			
Ag1···Cl2, Ag1···Cl2^{i}	3.2436 (8)		Ag1···Br2	3.2289 (8)		
Ag1···Cl1, Ag1···Cl1^{i}	3.3101 (10)		Ag1···Br4	3.3201 (7)		
			Ag1···Br3	3.3832 (7)		
Nitrate group bonds			**Nitrate group bonds**			
N2–O2	1.202(6)		N3–O1	1.242(6)		
N2–O1, N2–O1^{i}	1.249(3)		N3–O2	1.229(7)		
			N3–O3	1.213(6)		
< N2–O>	<1.233>		< N3–O>	<1.228>		
2,6–dichloropyridine bonds			**2,6–dibromopyridine bonds**			
Cl1–C1	1.730(3)		Br1–C1	1.877(5)	Br3–C6	1.888(5)
Cl2–C5	1.732(2)		Br2–C5	1.873(5)	Br4–C10	1.879(5)
<Cl–C>	<1.731>		<Br–C>	<1.875>	<Br–C>	<1.884>
N1–C1	1.336(3)		N1–C5	1.322(6)	N2–C6	1.334(6)
N1–C5	1.326(3)		N1–C1	1.337(6)	N2–C10	1.333(6)
< N–C>	<1.331>		< N–C>			<1.332>
C1–C2	1.367(4)		C1–C2	1.365(6)	C6–C7	1.358(8)
C2–C3	1.365(4)		C2–C3	1.378(7)	C7–C8	1.372(8)
C3–C4	1.378(4)		C3–C4	1.367(7)	C8–C9	1.357(9)
C4–C5	1.366(3)		C4–C5	1.376(7)	C9–C10	1.366(8)
<C–C>	<1.369>		<C–C>			<1.367>
Cl···Cl interactions			**Br···Br interactions**			
Cl2···Cl2^{v}	3.4415(14)		Br1···Br2^{ii}	3.6283(8)		
∠C5–Cl2···Cl2^{v}	145.63(10)		∠C1–Br1···Br2^{ii}	156.2(2)		
∠Cl2···Cl2^{v}–C5^{v}	145.62(10)		∠Br1^{vii}···Br2–C5	104.6(2)		
Cl1–Cl2^{iii}	*3.6117(11)*		Br1–Br1^{iii}	3.714(2)		
∠C1–Cl1–Cl^{iii}	*167.21(10)*		∠C1–Br1···Br1^{iii}	134.2(2)		
∠Cl1^{vi}···Cl2– C5	*99.42(9)*		∠Br1···Br1^{iii}–C1^{iii}	134.2(2)		
C–Cl···O halogen bonds			**C–Br···O halogen bonds**			
			Br4···O2^{v}	*3.367(5)*		
			∠C10–Br4···O2^{v}	*168.6(4)*		
			Br3···O1^{iv}	*3.412(4)*		
			∠C6–Br3···O1^{iv}	*161.1(4)*		
C–H···O bonds and interactions			**C–H···O bonds and interactions**			
H2···O1^{iv}	2.55		H4··· O3^{viii}	2.41		
∠CHO	146		∠CHO	149		
H3···O1^{vii}	2.52		H7···O2^{ii}	2.39		
∠CHO	128		∠CHO	169		
H4···O1^{vii}	2.73		H3···O1^{i}	2.50	*H2···O1^{i}*	*2.69*
∠CHO	118		∠CHO	118	*∠CHO*	*110*
H2···O2^{iv}	2.73					
∠CHO	161					
C–H···Cl interactions			**C–H···Br interactions**			
C–Cl···π interactions Cg1: 0.1571, 0.8296, 0.1454			**C–Br···π interactions** Cg1: 0.4822, 0.0702, –0.1252; Cg2: 0.1666, 0.2281, 0.2838			
Cl1···Cg1^{viii}	3.745(1)		Br4···Cg1^{vi}	3.959 (2)		
∠C1–Cl1···Cg1^{viii}	106.0(1)		∠C10–Br4···Cg1^{vi}	84.8(1)		
			Br4···Cg2^{v}	3.730(2)		
			∠C10–Br4···Cg2^{v}	89.6(1)		
π–stacking interactions			**π–stacking interactions**			
			Cg1···Cg1^{i}	3.735(3)		
Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) *x*, *y*+1, *z*; (iii) *x*−1/2, −*y*+1/2, *z*−1/2; (iv) −*x*+1, −*y*, −*z*; (v) −*x*+3/2, −*y*+1/2, −*z*+1; (vi) *x*+1/2, −*y*+1/2, *z*+1/2; (vii) *x*+1/2, *y*+1/2, *z*; (viii) 1−*x*, 1−*y*, −*z*.			Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*; (v) *x*, −*y*+3/2, *z*+1/2; (vi) *x*, −*y*+3/2, *z*−1/2; (vii) *x*−1, *y*, *z*; (viii) *x*, *y*, *z*+1;			

Table S3c. The bond-length geometry (Å, °) with the coordinating ligands and intermolecular interactions in **3**.

$[Ag(NO_3)(3,5\text{-}Cl_2py)_2]$ (3)							
Ag–N and Ag–O bonds		Σv_{ij} **(v.u.)**		**Ag–N and Ag–O bonds**		Σv_{ij} **(v.u.)**	
Ag1–N2	2.244 (4)	0.3437		Ag2–N3	2.226 (4)	0.3639	
Ag1–N1	2.288 (4)	0.3070		Ag2–N4	2.270 (4)	0.3228	
Ag1–O1	2.491 (4)	0.1742		Ag2–O4	2.514 (4)	0.1633	
Ag1–O4	2.706 (4)	0.1410		Ag2–O3^{i}	2.758 (4)	0.0839	
	CN=4	0.9659			CN=4	0.9339	
< Ag–N> < Ag–O>	<2.27> <2.60>			< Ag–N> < Ag–O>	<2.25> <2.64>		
Ag···O interactions				**Ag···O interactions**			
Ag1···O5	2.840 (4)	0.0965		Ag2···O1^{i}	2.786 (4)	0.0779	
Ag1···O2	3.017 (4)	0.0417		Ag2···O6	3.023 (4)	0.0410	
	CN=4+2	1.1041			CN=4+2	1.0528	
< Ag···O>	< 2.93>			< Ag···O>	< 2.90>		
Nitrate group bonds							
N5–O1	1.249 (5)			N6–O4	1.257 (5)		
N5–O2	1.233 (5)			N6–O5	1.227 (5)		
N5–O3	1.238 (4)			N6–O6	1.235 (5)		
< N5–O>	<1.24>			< N6–O>	<1.24>		
3,5–dichloropyridine bonds							
Cl1–C2	1.726 (4)	Cl3–C7	1.723 (5)	Cl5–C12	1.730 (4)	Cl7–C17	1.741(4)
Cl2–C4	1.732 (4)	Cl4–C9	1.739 (5)	Cl6–C14	1.728 (4)	Cl8–C19	1.730(4)
<Cl–C>	<1.73>	<Cl–C>	<1.73>	<Cl–C>	<1.73>	<Cl–C>	<1.74>
N1–C1	1.337 (5)	N2–C6	1.341 (5)	N3–C11	1.340 (6)	N4–C16	1.344(6)
N1–C5	1.336 (5)	N2–C10	1.326 (6)	N3–C15	1.336 (5)	N4–C20	1.341(5)
< N1–C>	<1.33>	< N2–C>	<1.33>	< N3–C>	<1.34>	< N4–C>	<1.34>
C1–C2	1.377 (6)	C6–C7	1.357 (6)	C11–C12	1.356 (7)	C16–C17	1.357(6)
C2–C3	1.374 (6)	C7–C8	1.384 (6)	C12–C13	1.380 (6)	C17–C18	1.377(6)
C3–C4	1.373 (6)	C8–C9	1.370 (6)	C13–C14	1.371 (6)	C18–C19	1.362(6)
C4–C5	1.382 (6)	C9–C10	1.378 (6)	C14–C15	1.371 (6)	C19–C20	1.379(6)
< C–C>	<1.38>	<C–C>	<1.37>	<C–C>	<1.37>	<C–C>	<1.37>
Cl···Cl interactions							
Cl1···Cl2^{ii}	3.311 (2)	Cl3···Cl4^{ii}	3.417 (2)	Cl5···Cl6^{i}	3.300 (2)		
∠C2–Cl1···Cl2^{ii}	116.0 (2)	∠C7–Cl3···Cl4^{ii}	111.6 (2)	∠C12–Cl5···Cl6^{i}	173.2(2)		
∠Cl1^{i}···Cl2–C4	171.8 (2)	∠Cl3^{i}···Cl4–C9	168.7 (2)	∠Cl5^{ii}···Cl6–C14	116.6 (2)		
Cl6···Cl7^{iii}	3.507 (2)	Cl1···Cl3^{iii}	3.557 (2)	Cl7···Cl8^{ii}	3.396 (2)		
∠C14–Cl6···Cl7^{iii}	163.3 (2)	∠C2–Cl1···Cl3^{iii}	160.3 (2)	∠C17–Cl7···Cl8^{ii}	112.3 (2)		
∠Cl6^{viii}···Cl7–C17	94.9 (2)	∠Cl1^{viii}···Cl3–C7	95.9 (2)	∠Cl7^{i}···Cl8– C19	168.5 (2)		
C–Cl···O interactions							
C–H···O bonds and interactions							
H1···O1	2.53	H10···O3^{i}	2.32	H16···O4	2.61		
∠C1–H1···O1	132	∠ C10–H10···O3^{i}	173	∠C16–H16···O4	132		
H3···O2^{iv}	2.56	H11···O5^{i}	2.38	H18···O6^{vi}	2.64		
∠C3–H3···O2^{iv}	133	∠ C11–H11···O5^{i}	171	∠C18–H18···O6^{vi}	135		
H5···O3^{i}	2.39	H15···O6	2.49				
∠C5–H5···O3^{i}	169	∠ C15–H15···O6	134				
H6···O2	2.51	H20···O5^{i}	2.42				
∠C6–H6···O2	137	∠C20–H20···O5^{i}	167				
C–H···Cl interactions							
H8···Cl1^{v}	2.80						
∠C8–H8···Cl1^{v}	149						
H18···Cl6^{v}	2.86						
∠C18–H18···Cl6^{v}	140						
C–Cl···π interactions	Cg1: 0.3612, 0.1179, 0.5077; Cg2: 0.4916, 0.1332, 0.0046			Cg3: 0.8202, 0.3641, 0.5013; Cg4: 0.9383, 0.3811, –0.0039			
Cl2···Cg3	3.624 (3)			Cl5···Cg3^{viii}	3.938 (3)		
∠C4–Cl2···Cg3	101.4 (1)			∠C12–Cl5···Cg3^{viii}	117.9 (1)		
Cl4···Cg4	3.846 (3)			Cl6···Cg3^{ix}	3.979 (3)		
∠C9–Cl4···Cg4	98.8 (1)			∠C14–Cl6···Cg3^{ix}	91.0 (1)		
Cl5···Cg1^{i}	3.903 (3)			Cl8···Cg2^{i}	3.669 (3)		
∠C12–Cl5···Cg1^{i}	101.3 (1)			∠C19–Cl8···Cg2^{i}	104.45 (1)		
π–stacking interactions							
Cg1··· Cg1^{iv}	3.726 (3)			Cg4···Cg4^{x}	3.595 (3)		
Cg2··· Cg2^{vii}	3.675 (3)						
Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) *x*, *y*, *z*+1; (iv) −*x*+1, −*y*, −*z*+1; (v) *x*, *y*, *z*−1; (vi) −*x*, −*y*+1, −*z*; (vii) −*x*+1, −*y*, −*z*; (viii) −*x*−1, −*y*+1, −*z*+1; (ix) −*x*, −*y*+1, −*z*+1; (x) −*x*, −*y*+1, −*z*.							

Table S3d. The bond-length geometry (Å, °) with the coordinating ligands and intermolecular interactions in **6**.

$[Ag(NO_3)(3,5\text{-}Br_2py)_2]$ (6)		
Ag–N and Ag–O bonds	Σv_{ij} **(v.u.)**	

Ag1–N1	2.249(6)	0.3415	
Ag1–N2	2.248(6)	0.3402	
Ag1–O3	2.433(7)	0.2026	
Ag1–O3^{i}	2.520(6)	0.1599	
	CN=4	1.0442	
< Ag–N> < Ag–O>	<2.245> <2.465>		
Ag···O interactions			
Ag1···O1^{i}	2.756(7)	0.0845	
Ag1···O2	2.965(7)	0.0480	
	CN=4+2	1.1767	
Nitrate group bonds			
N3–O1	1.220(10)		
N3–O2	1.234(9)		
N3–O3	1.248(8)		
< N3–O>	<1.234>		
3,5–dibromopyridine bonds			
Br1–C4	1.885(7)	Br3–C9	1.880(8)
Br2–C2	1.865(8)	Br4–C7	1.895(7)
<Br–C>	<1.875>	<Br–C>	<1.888>
N1–C1	1.327(9)	N2–C10	1.337(10)
N1–C5	1.329(9)	N2–C6	1.327(10)
< N1–C>	<1.328>	< N2–C>	<1.332>
C1–C2	1.387(11)	C6–C7	1.366(10)
C2–C3	1.379(10)	C7–C8	1.379(11)
C3–C4	1.370(11)	C8–C9	1.371(11)
C4–C5	1.353(11)	C9–C10	1.379(11)
<C–C>	<1.373>	<C–C>	<1.374>
Br···Br interactions			
Br3···Br4^{iv}	*3.7329(13)*		
∠C9–Br3···Br4^{iv}	*91.9(5)*		
∠Br3^{v}··· Br4– C7	*177.7(3)*		
C–Br···O halogen bonds			
Br1···O2^{ii}	3.010(5)		
∠C4−Br1···O2 ^{ii}	162.1 (3)		
Br2···O2^{iii}	3.246(7)		
∠C2−Br2···O2^{iii}	160.0 (5)		
C–H···O bonds and interactions			
H8···O1^{v}	2.40		
∠C8−H8···O1^{v}	152		
C–Br···π interactions Cg1: 0.8348, 0.5299, 0.4501; Cg2: 0.8162, 0.0823, 0.2678			
Br1…Cg2^{vi}	3.808(3)		
∠C4–Br1…Cg2^{vi}	115		
Br2…Cg2^{vii}	3.858(3)		
∠C2–Br2…Cg2^{vii}	76		
π–stacking interactions			
Cg2···Cg1^{viii}	4.346(4)		
Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) −*x*+1/2, −*y*+1, *z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+1/2 (iv) −*x*+1/2, −*y*+2, *z*+1/2 (v) −*x*+1, *y*+1/2, −*z*+1/2 (vi) *x*−1/2, −*y*+3/2, −*z*+1; (vii) −*x*, *y*−1/2, −*z*+1/2; (viii) $-x, y+1/2, -z+1/2$.			

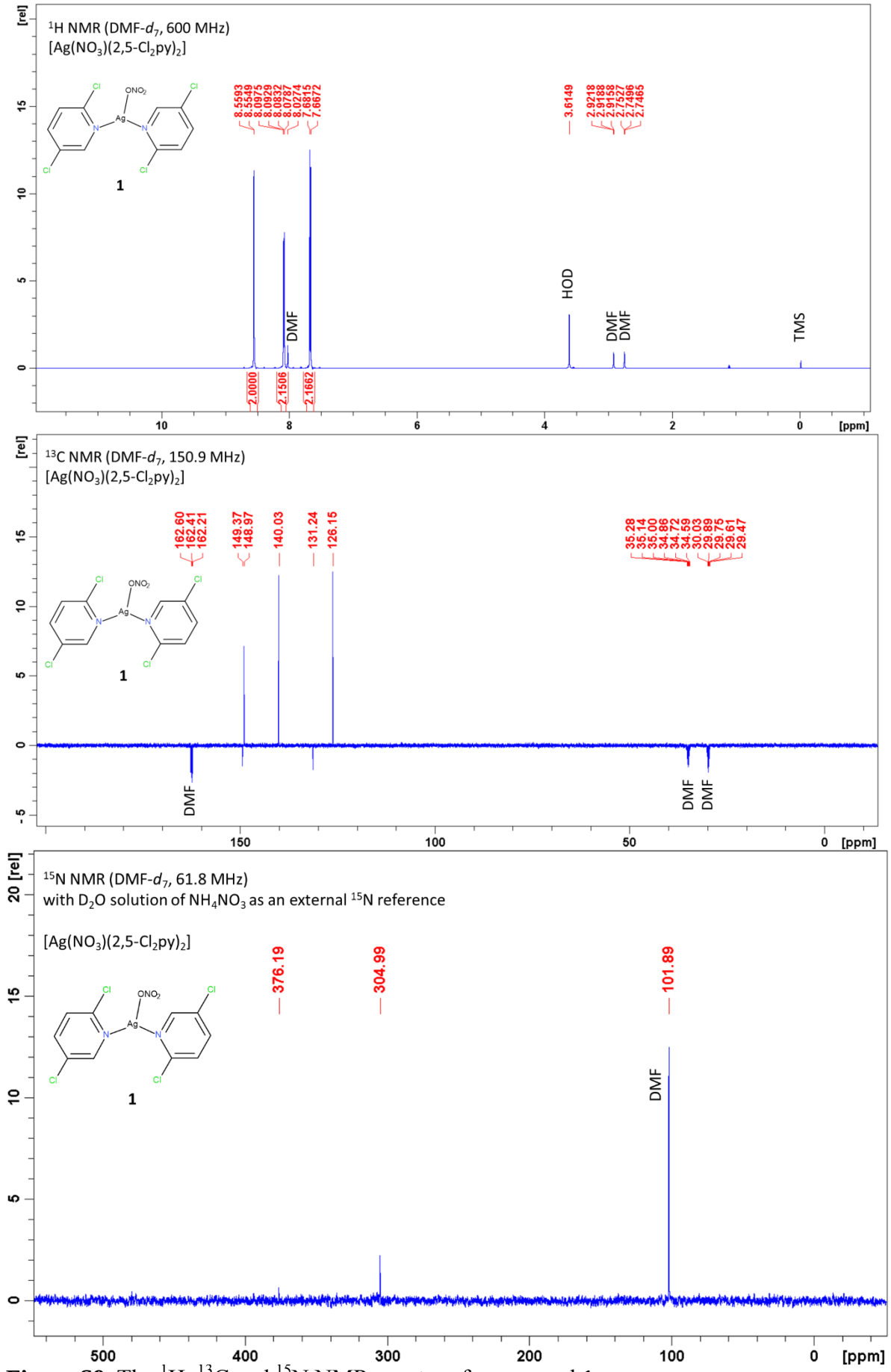

Figure S9. The ^{1}H, ^{13}C and ^{15}N NMR spectra of compound **1**.

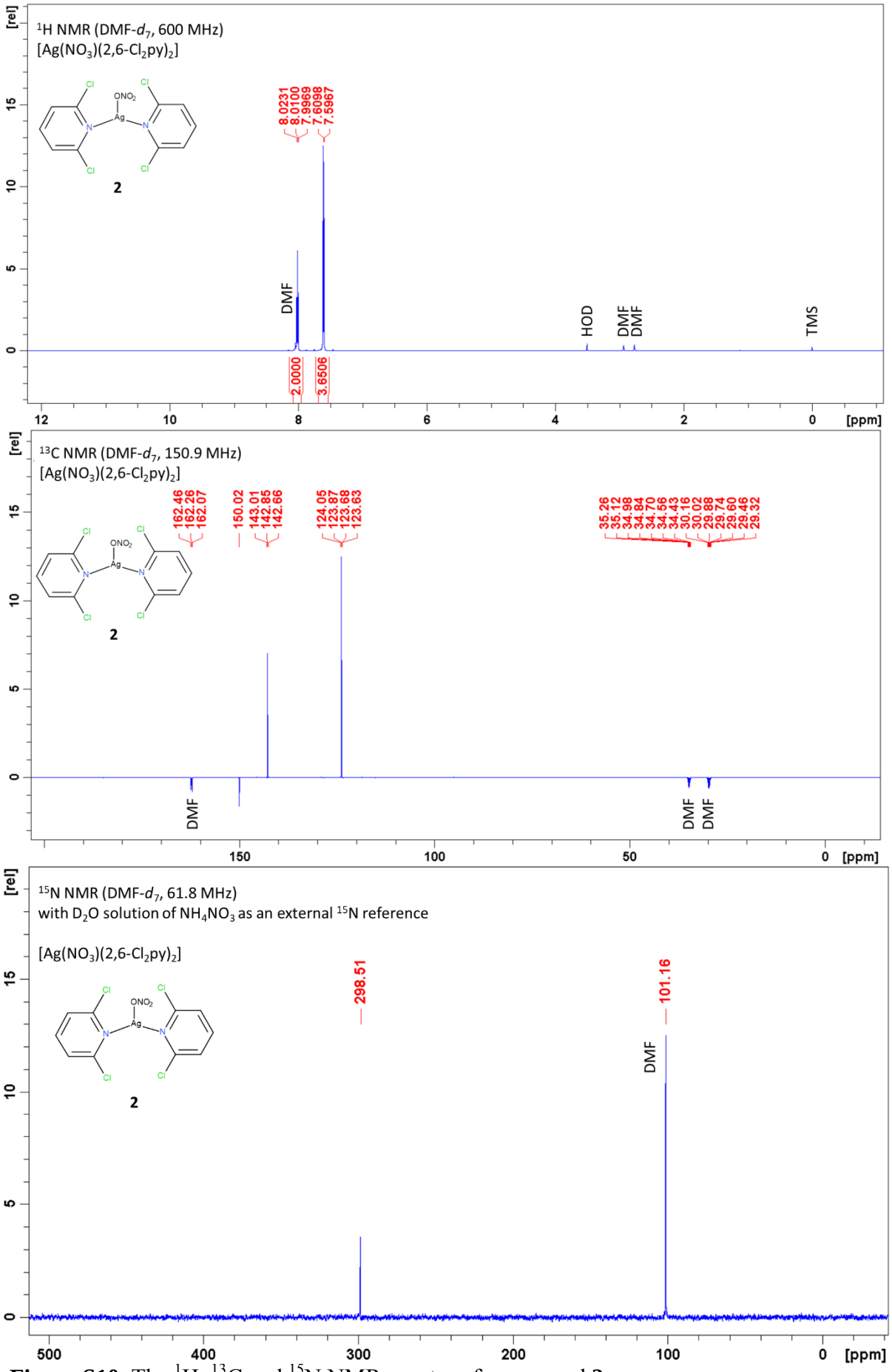

Figure S10. The ^{1}H, ^{13}C and ^{15}N NMR spectra of compound **2**.

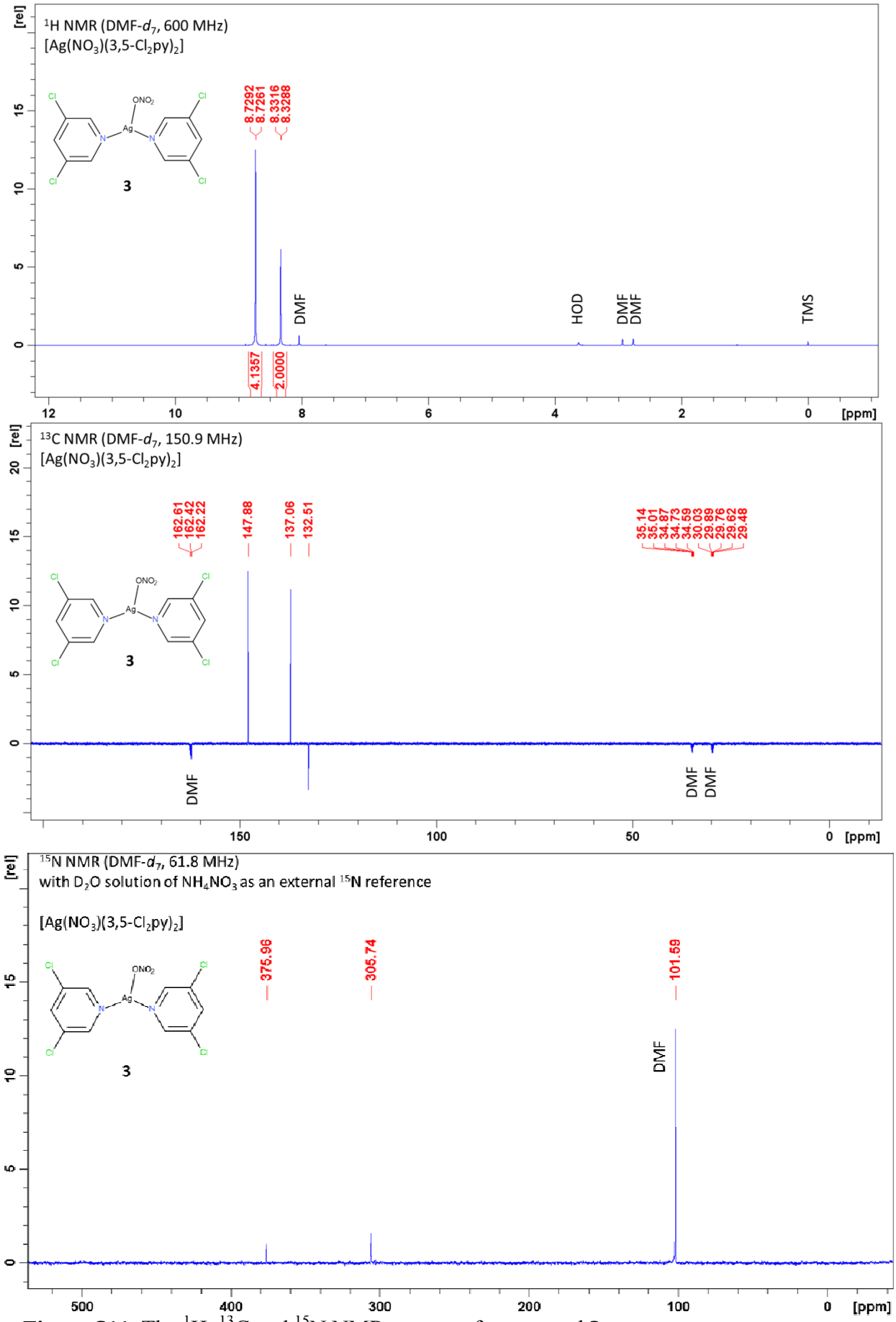

Figure S11. The ^{1}H, ^{13}C and ^{15}N NMR spectra of compound **3**.

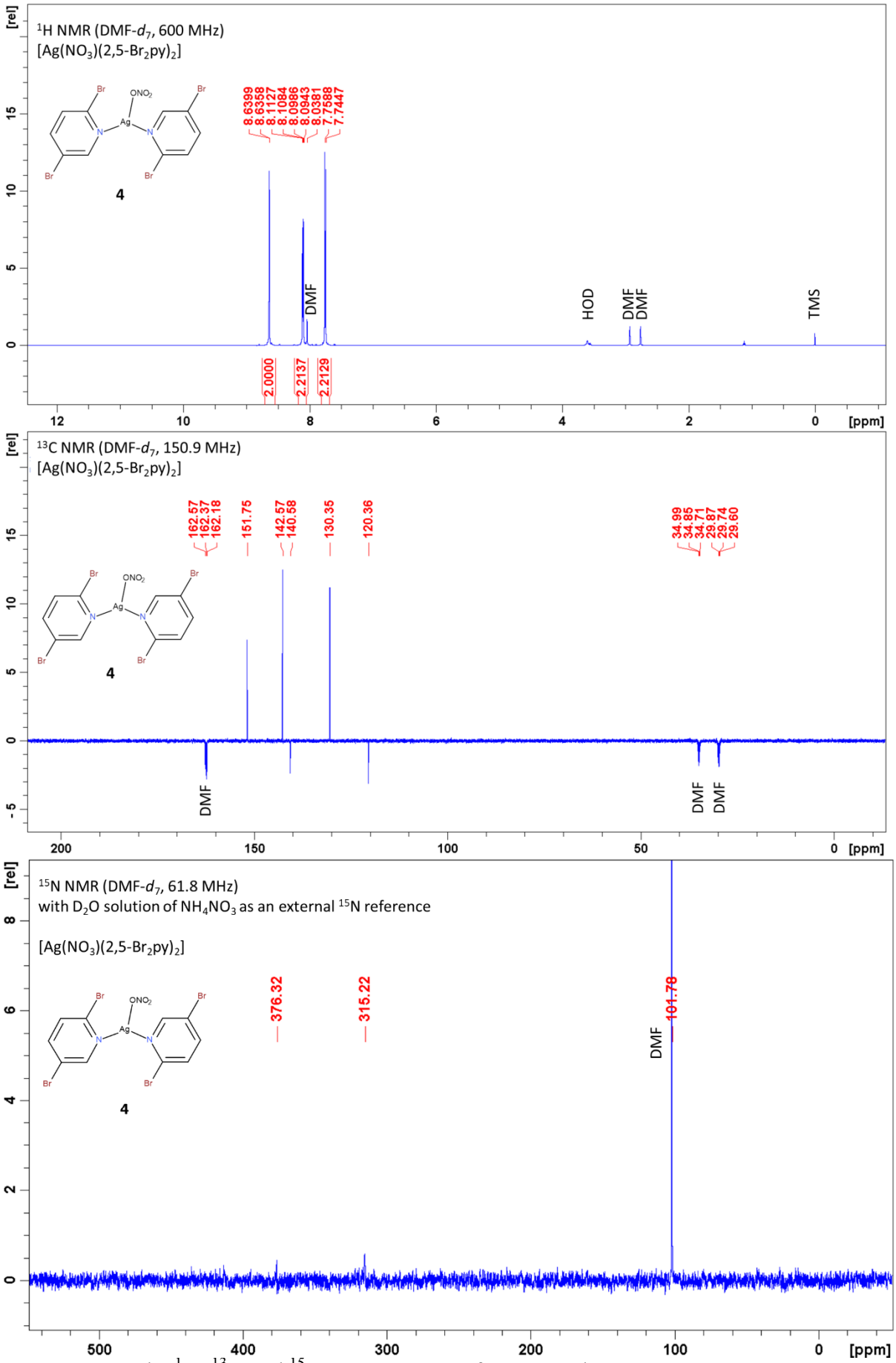

Figure S12. The ^{1}H, ^{13}C and ^{15}N NMR spectra of compound **4**.

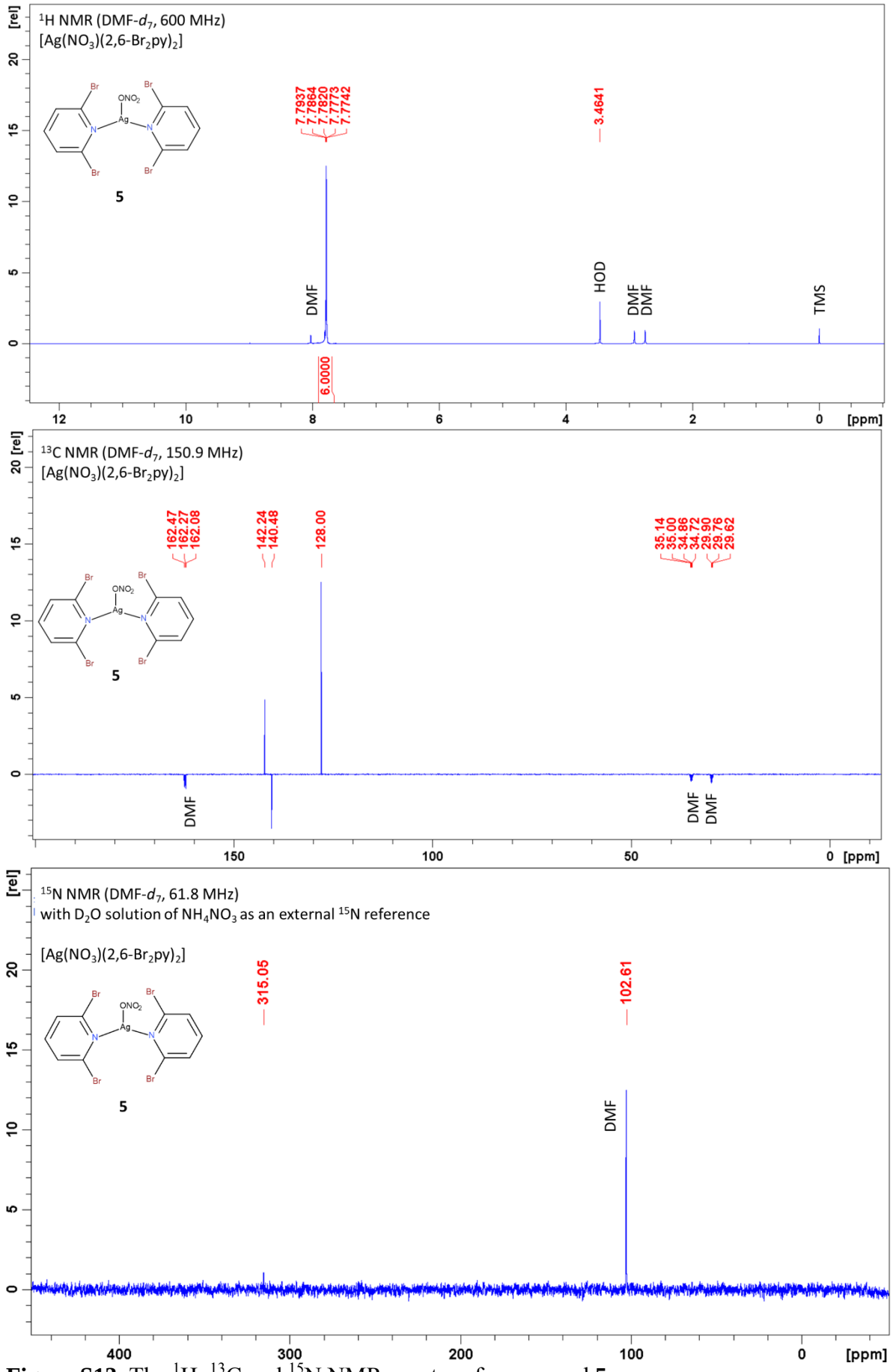

Figure S13. The ^{1}H, ^{13}C and ^{15}N NMR spectra of compound **5**.

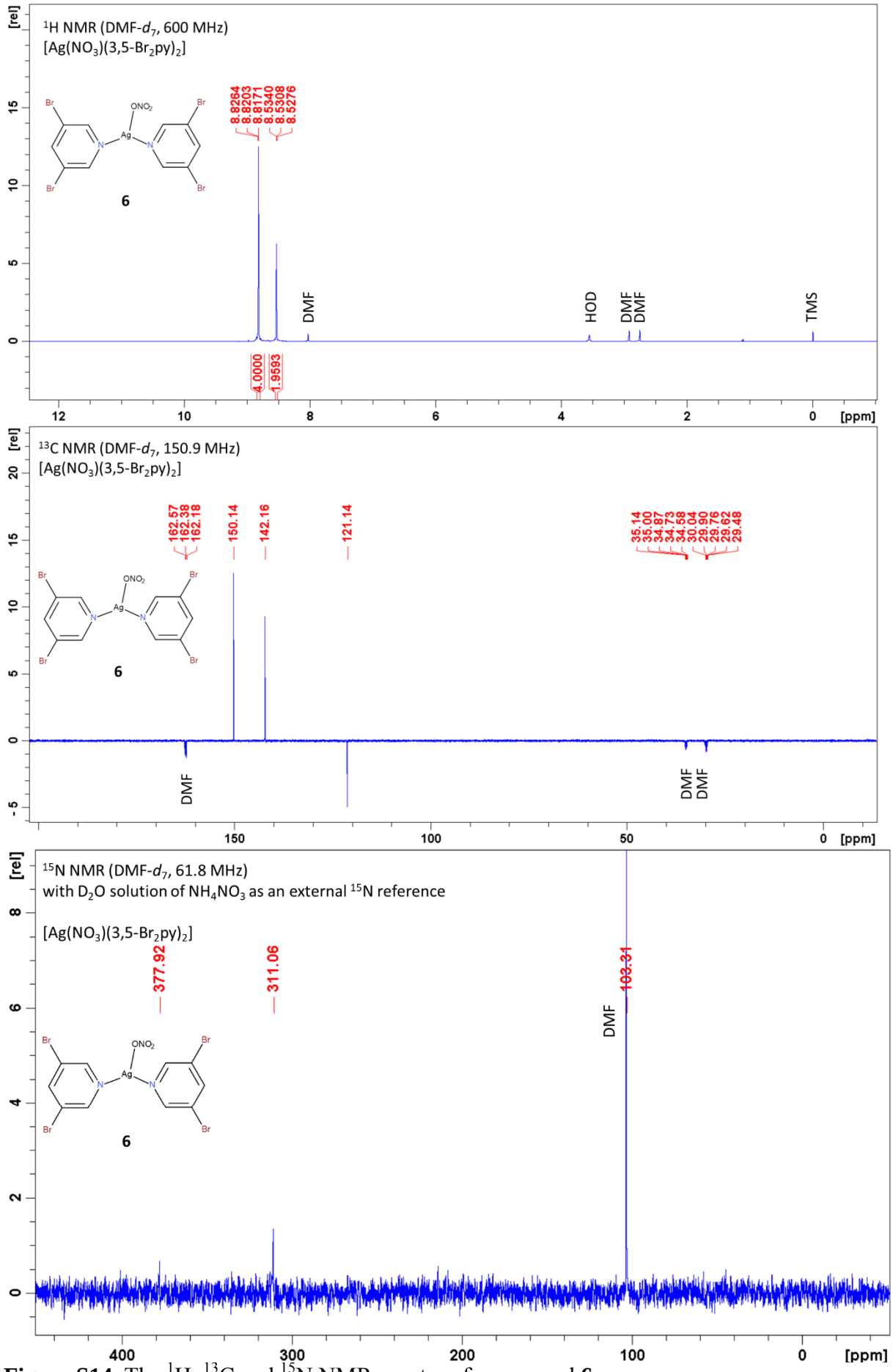

Figure S14. The ^{1}H, ^{13}C and ^{15}N NMR spectra of compound **6.**

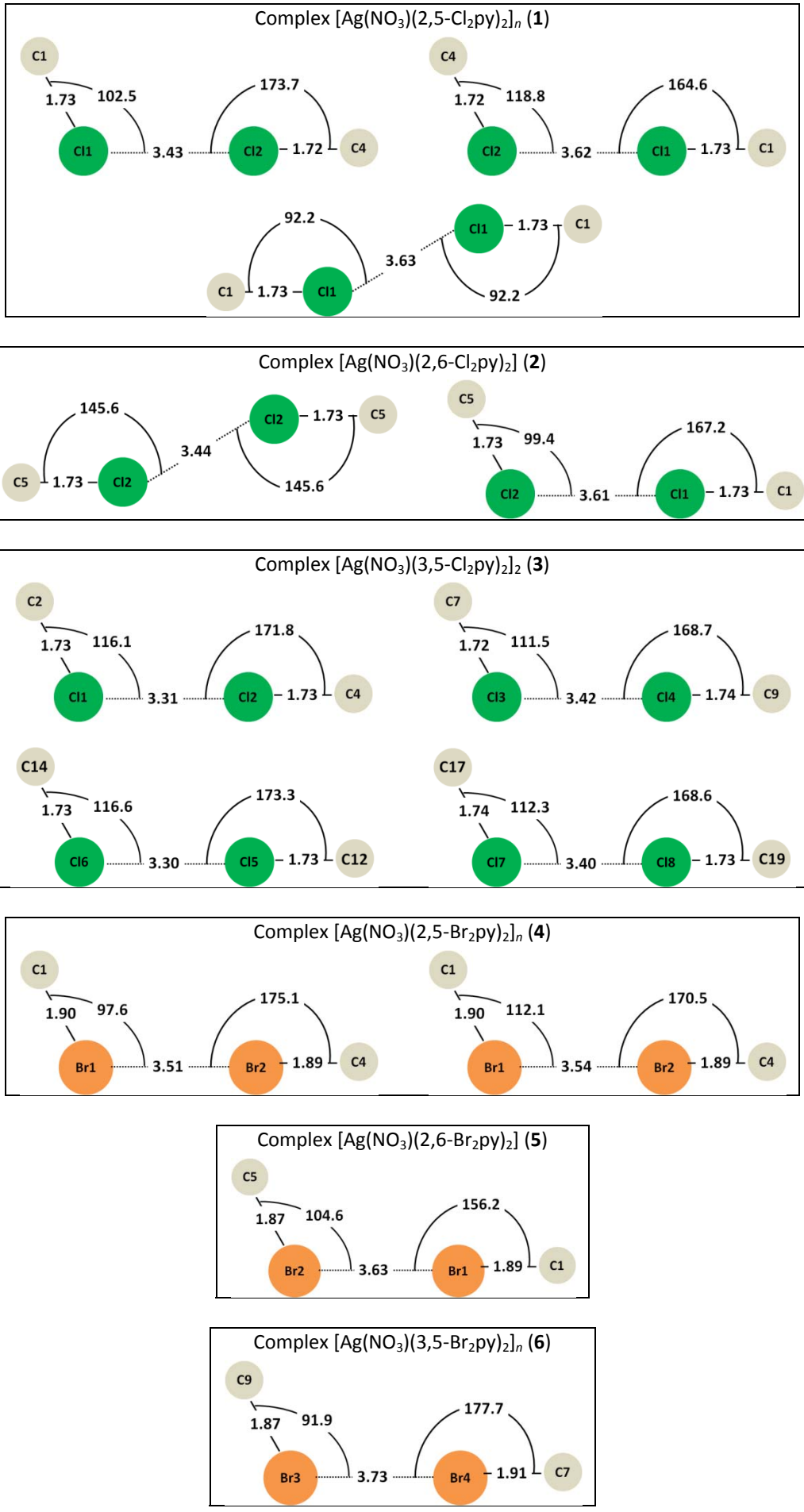

Figure S15. Graphical representation of the relevant geometric parameters describing halogen···halogen interactions in **1**–**6**.

Details of the preparation and experimental characterization of complexes 1–6

Preparation of complexes

All chemicals for the syntheses were of reagent grade, purchased from commercial sources (Aldrich, Acros, Ega-Chemie) and used as received without further purification. Deuterated *N*,*N*-dimethylformamide (DMF-d_7) for NMR spectroscopy was purchased from Euriso-Top.

General procedure. Ethanol solution of the corresponding dihalopyridine (2 mmol in 15–20 mL) was added dropwise with moderate stirring to an aqueous solution of silver(I) nitrate (1 mmol in 5 mL). The reaction mixture was left to stand at room temperature to crystallize. After a while, colourless crystals were obtained. They were carefully filtered off, washed with cold ethanol and dried in a desiccator in the dark.

$[Ag(NO_3)(2,5\text{-}Cl_2py)_2]_n$ (1). From a reaction mixture of 2,5-dichloropyridine (0.36 g, 2 mmol in 5 mL of EtOH) and $AgNO_3$ (0.17 g, 1 mmol in 5 mL of water) colourless crystals of $[Ag(NO_3)(2,5\text{-}Cl_2py)_2]_n$ were isolated. Yield: 0.20 g (38%). *Anal.* Calc. for $C_{10}H_6AgCl_4N_3O_3$ (465.8): C, 25.78; H, 1.30; N, 9.02%. Found: C, 25.90; H, 1.18; N, 8.90%. FT-IR (KBr pellets): ν_{max}/cm^{-1} = 3046 (m), 2395 (w), 1956 (w), 1831 (w), 1763 (m), 1630 (w, br), 1559 (m-s), 1382 (vs, br), 1276 (m), 1112 (s), 1011 (s), 918 (m), 836 (s), 769 (w), 722 (m), 629 (m), 544 (m-s), 491 (m), 412 (m). ^{1}H NMR (600.130 MHz; DMF-d_7): δ (ppm) = 8.56 (2H, d, $^4J_{H,H}$ = 2.6 Hz, H-6), 8.09 (2H, dd, $^3J_{H,H}$ = 8.5 Hz, $^4J_{H,H}$ = 2.7 Hz, H-4), 7.68 (2H, d, $^3J_{H,H}$ = 8.6 Hz, H-3). ^{13}C NMR (150.903 MHz; DMF-d_7): δ (ppm) = 149.4 (2C, C-2), 149.0 (2C, C-6), 140.0 (2C, C-4), 131.2 (2C, C-5), 126.1 (2C, C-3). ^{15}N NMR (61.834 MHz; DMF-d_7): δ (ppm) = 376.2 (1N, NO_3^-), 305.0 (2N, N-py). ESI$^+$-MS (MeOH): *m/z* = 107 Ag^+, 148 $[2,5\text{-}Cl_2py + H]^+$, 254 $[Ag(2,5\text{-}Cl_2py)]^+$, 401 $[Ag(2,5\text{-}Cl_2py)_2]^+$. ESI$^-$-MS (MeOH): *m/z* = 62 $[NO_3]^-$, 230.5 $[Ag(NO_3)_2]^-$, 399.3 $[Ag_2(NO_3)_3]^-$.

$[Ag(NO_3)(2,6\text{-}Cl_2py)_2]$ (2). From a reaction mixture with 2,6-dichloropyridine (0.36 g, 2 mmol in 11.5 mL of EtOH) and $AgNO_3$ (0.17 g, 1 mmol in 5 mL of water) colourless crystals of $[Ag(NO_3)(2,6\text{-}Cl_2py)_2]$ were isolated. Yield: 0.12 g (23%). *Anal.* Calc. for $C_{10}H_6AgCl_4N_3O_3$ (465.8): C, 25.78; H, 1.30; N, 9.02%. Found: C, 24.67; H, 0.91; N, 8.70%. FT-IR (KBr pellets): ν_{max}/cm^{-1} = 3117 (w), 3049 (m), 1632 (w), 1561 (s), 1424 (vs), 1382 (vs, br), 1164 (m), 1139 (m), 1081 (w), 987 (m), 793 (s), 666 (m), 455 (w), 377 (w). ^{1}H NMR (600.130 MHz; DMF-d_7): δ (ppm) = 7.99 (2H, t, $^3J_{H,H}$ = 8.1 Hz, H-4), 7.59 (4H, d, $^3J_{H,H}$ = 7.8 Hz, H-3, H-5). ^{13}C NMR (150.903 MHz; DMF-d_7): δ(ppm) = 150.0 (4C, C-2, C-6), 142.9 (2C, C-4), 123.9 (4C, C-3, C-5). ^{15}N NMR (61.834 MHz; DMF-d_7): δ (ppm) = 298.5 (2N, N-py). NO_3^- signal was not detected. ESI$^+$-MS (MeOH): *m/z* = 107 $[Ag^+]$, 254 $[Ag(2,6\text{-}Cl_2py)]^+$, 401 $[Ag(2,6\text{-}Cl_2py)_2]^+$. ESI$^-$-MS (MeOH): *m/z* = 62 $[NO_3]^-$, 230 $[Ag(NO_3)_2]^-$, 399 $[Ag_2(NO_3)_3]^-$.

$[Ag(NO_3)(3,5\text{-}Cl_2py)_2]_2$ (3). From a reaction mixture with 3,5-dichloropyridine (0.36 g, 2 mmol in 6 mL of EtOH) and $AgNO_3$ (0.17 g, 1 mmol in 5 mL of water) colourless crystals of $[Ag(NO_3)(3,5\text{-}Cl_2py)_2]_2$ were isolated. Yield: 0.23 g (43%). *Anal.* Calc. for $C_{10}H_6AgCl_4N_3O_3$ (465.8): C, 25.78; H, 1.30; N, 9.02%. Found: C, 24.37; H, 0.93; N, 8.90%. FT-IR (KBr pellets): ν_{max}/cm^{-1} = 3055 (m), 3024 (m), 1763 (w), 1627 (w), 1558 (m), 1382 (vs, br), 1295 (m), 1112 (m), 1035 (w), 881 (w-m), 810 (m), 690 (m), 448 (w), 399 (w). ^{1}H NMR (600.130 MHz; DMF-d_7): δ (ppm) = 8.73 (4H, d, $^4J_{H,H}$ = 1.9 Hz, H-2, H-6), 8.33 (2H, t, $^4J_{H,H}$ = 1.7 Hz, H-4). ^{13}C NMR (150.903 MHz; DMF-d_7): δ (ppm) = 147.9 (4C, C-2, C-6), 137.1 (2C, C-4), 132.5 (4C, C-3, C-5). ^{15}N NMR (61.834 MHz; DMF-d_7): δ (ppm) = 376.0 (1N, NO_3^-), 305.7 (2N, N-py). ESI^+-MS (MeOH): *m/z* = 107 [Ag^+], 148 [3,5-Cl_2py + H]$^+$, 254 [Ag(3,5-Cl_2py)]$^+$. ESI^--MS (MeOH): *m/z* = 62 [NO_3]$^-$, 230 [$Ag(NO_3)_2$]$^-$, 399 [$Ag_2(NO_3)_3$]$^-$.

$[Ag(NO_3)(2,5\text{-}Br_2py)_2]_n$ (4). From a reaction mixture with 2,5-dibromopyridine (0.47 g, 2 mmol in 9.5 mL of EtOH) and $AgNO_3$ (0.17 g, 1 mmol in 5 mL of water) colourless crystals of $[Ag(NO_3)(2,5\text{-}Br_2py)_2]_n$ were isolated. Yield: 0.35 g (55%). *Anal.* Calc. for $C_{10}H_6AgBr_4N_3O_3$ (643.6): C, 18.66; H, 0.94; N, 6.53%. Found: C, 18.74; H, 0.94; N, 6.38%. FT-IR (KBr pellets): ν_{max}/cm^{-1} = 3025 (m), 1629 (w), 1555 (m), 1439 (m-s), 1384 (vs, br), 1093 (m-s), 1000 (m), 831 (m), 715 (w), 626 (w), 482 (w), 423 (w). ^{1}H NMR (600.130 MHz; DMF-d_7): δ (ppm) = 8.63 (2H, d, $^4J_{H,H}$ = 2.2 Hz, H6), 8.09 (2H, dd, $^3J_{H,H}$ = 8.8 Hz, $^4J_{H,H}$ = 2.6 Hz, H4), 7.74 (2H, d, $^3J_{H,H}$ = 8.8 Hz, H-3). ^{13}C NMR (150.903 MHz; DMF-d_7): δ (ppm) = 151.7 (2C, C-6), 142.6 (2C, C-4), 140.6 (2C, C-2), 130.3 (2C, C3), 120.4 (2C, C5). ^{15}N NMR (61.834 MHz; DMF-d_7): δ (ppm) = 376.3 (1N, NO_3^-), 315.2 (2N, N-py). ESI^+-MS (MeOH): *m/z* = 107 Ag^+, 342 [Ag(2,5-Br_2py)]$^+$, 577 [Ag(2,5-Br_2py)$_2$]$^+$. ESI^--MS (MeOH): *m/z* = 62 [NO_3]$^-$, 230 [$Ag(NO_3)_2$]$^-$, 399 [$Ag_2(NO_3)_3$]$^-$.

$[Ag(NO_3)(2,6\text{-}Br_2py)_2]$ (5). From a reaction mixture with 2,6-dibromopyridine (0.47 g, 2 mmol in 8 mL of EtOH) and $AgNO_3$ (0.17 g, 1 mmol in 5 mL of water) colourless crystals of $[Ag(NO_3)(2,6\text{-}Br_2py)_2]$ were isolated. Yield: 0.54 g (84%). *Anal.* Calc. for $C_{10}H_6AgBr_4N_3O_3$ (643.6): C, 18.66; H, 0.94; N, 6.53%. Found: C, 18.08; H, 0.89; N, 6.48%. FT-IR (KBr pellets): ν_{max}/cm^{-1} = 3066 (w), 2922 (w), 1738 (w), 1632 (w), 1576 (m), 1462 (m), 1384 (vs, bs), 1193 (m), 1079 (m), 1010 (m), 931 (w), 787 (m), 693 (m), 618 (w), 395 (w). ^{1}H NMR (600.130 MHz; DMF-d_7): δ (ppm) = 7.80–7.77 (6H, m, H-3, H-4, H-5). ^{13}C NMR (150.903 MHz; DMF-d_7): δ (ppm) = 142.2 (2C, C-4), 140.5 (4C, C-2, C-6), 128.0 (4C, C-3, C-5). ^{15}N NMR (61.834 MHz; DMF-d_7): δ (ppm) = 315.0 (2N, N-py). NO_3^- signal was not detected. ESI^+-MS (MeOH): *m/z* = 107 Ag^+, 342 [Ag(2,6-Br_2py)]$^+$, 577 [Ag(2,6-Br_2py)$_2$]$^+$. ESI^--MS (MeOH): *m/z* = 62 [NO_3]$^-$, 230 [$Ag(NO_3)_2$]$^-$, 399 [$Ag_2(NO_3)_3$]$^-$.

$[Ag(NO_3)(3,5\text{-}Br_2py)_2]_n$ (6). From a reaction mixture with 3,5-dibromopyridine (0.47 g, 2 mmol in 4.5 mL of EtOH) and $AgNO_3$ (0.17 g, 1 mmol in 5 mL of water) colourless crystals of $[Ag(NO_3)(3,5\text{-}Br_2py)_2]_n$ were isolated. Yield: 0.54 g (84%). *Anal.* Calc. for $C_{10}H_6AgBr_4N_3O_3$ (643.6): C, 18.66; H, 0.94; N, 6.53%. Found: C, 18.78; H, 0.71; N, 6.43%. FT-IR (KBr pellets): ν_{max}/cm^{-1} = 3041 (m), 3010 (m), 1734 (w), 1632 (m, br), 1544 (s), 1384 (vs, br), 1299 (s), 1086 (m), 1018 (m), 933 (w), 875 (m-s), 819 (w), 759 (s), 683 (s). ^{1}H NMR (600.130 MHz; DMF-d_7): δ (ppm) = 8.82 (4H, d, $^3J_{H,H}$ = 1.9 Hz, H-2, H-6), 8.53 (2H, t, $^3J_{H,H}$ = 1.9 Hz, H-4). ^{13}C NMR (150.903 MHz; DMF-d_7): δ (ppm) = 150.1 (4C, C-2, C-6), 142.2 (2C, C-4), 121.1 (4C, C-3, C-5). ^{15}N NMR (61.834 MHz; DMF-d_7): δ (ppm) = 378.1 (1N, NO_3^-), 311.2 (2N, N-py). ESI^+-MS (MeOH): *m/z* = 107 Ag^+, 342 $[Ag(3,5\text{-}Br_2py)]^+$, 578 $[Ag(3,5\text{-}Br_2py)_2]^+$. ESI^--MS (MeOH): *m/z* = 62 $[NO_3]^-$, 230 $[Ag(NO_3)_2]^-$, 399 $[Ag_2(NO_3)_3]^-$.

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-248.23106
Thermal Correction to Gibbs Free Energy (in a.u.)	0.062092

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	1	0	-2.066988	-1.301415	0.000026
3	6	0	-1.196936	0.671191	-0.000057
4	6	0	0.000041	1.383879	-0.000024
5	6	0	1.196976	0.671118	0.000080
6	6	0	1.143424	-0.720458	-0.000281
7	7	0	-0.000044	-1.420308	0.000062
8	1	0	-2.160038	1.179617	-0.000094
9	1	0	0.000078	2.473979	0.000038
10	1	0	2.160102	1.179500	0.000355
11	1	0	2.066907	-1.301542	0.000338

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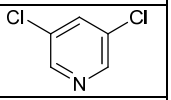
Ligand:	
Total electronic energy (in a.u.)	-1167.43496
Thermal Correction to Gibbs Free Energy (in a.u.)	0.038518

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.148473	1.379596	0.000170
2	1	0	2.073600	1.954559	0.000330
3	6	0	1.178796	-0.011636	-0.000361
4	6	0	0.000034	-0.745765	-0.000446
5	6	0	-1.178575	-0.011454	-0.000456
6	6	0	-1.148297	1.379738	-0.000756
7	7	0	0.000135	2.061674	0.000490
8	17	0	2.719972	-0.836806	0.000138
9	1	0	-0.000037	-1.834053	-0.000286
10	17	0	-2.720191	-0.836716	0.000291
11	1	0	-2.073368	1.954782	0.000332

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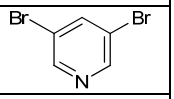
Ligand:	
Total electronic energy (in a.u.)	-5395.40430
Thermal Correction to Gibbs Free Energy (in a.u.)	0.035149

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000034	2.379920	0.000140
2	6	0	1.148532	1.697820	0.000226
3	6	0	1.181933	0.305983	-0.000101
4	6	0	-0.000022	-0.425479	-0.000280
5	1	0	-0.000112	-1.513850	-0.000298
6	6	0	-1.181970	0.306077	-0.000260
7	6	0	-1.148544	1.697870	-0.000410
8	1	0	-2.069599	2.280625	0.000223
9	1	0	2.069623	2.280521	0.000317
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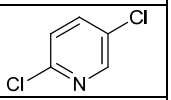
Ligand:	
Total electronic energy (in a.u.)	-1167.43998
Thermal Correction to Gibbs Free Energy (in a.u.)	0.038357

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.714749	-1.178300	0.000018
2	6	0	0.624073	-1.168735	0.000008
3	6	0	1.348465	0.016445	0.000005
4	6	0	0.687829	1.240704	0.000007
5	1	0	1.236685	2.180729	-0.000006
6	6	0	-0.701185	1.230728	0.000016
7	6	0	-1.330132	-0.010659	0.000042
8	1	0	-1.271400	2.156394	0.000002
9	17	0	-3.087510	-0.060468	-0.000021
10	1	0	1.126049	-2.135245	-0.000006
11	17	0	3.095605	-0.045689	-0.000013

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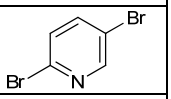
Ligand:	
Total electronic energy (in a.u.)	-5395.40814
Thermal Correction to Gibbs Free Energy (in a.u.)	0.035013

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.715105	-1.157823	0.000300
2	6	0	0.623696	-1.147455	0.000003
3	6	0	1.352106	0.036614	0.000046
4	6	0	0.687765	1.259272	0.000081
5	1	0	1.228337	2.204136	-0.000047
6	6	0	-0.702126	1.249045	0.000216
7	6	0	-1.334145	0.008620	0.000607
8	1	0	-1.265941	2.178392	0.000045
9	1	0	1.119967	-2.116963	0.000057
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11	35	0	3.246687	-0.033747	-0.000083

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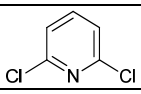
Ligand:	
Total electronic energy (in a.u.)	-1167.44423
Thermal Correction to Gibbs Free Energy (in a.u.)	0.038224

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	-0.688730	-0.000170
2	6	0	-1.124793	0.009230	0.000366
3	6	0	-1.204538	1.395609	0.000166
4	6	0	-0.000005	2.093572	0.000058
5	1	0	-0.000003	3.182787	0.000205
6	6	0	1.204538	1.395607	-0.000185
7	6	0	1.124802	0.009237	-0.000712
8	1	0	2.163517	1.906921	-0.000027
9	1	0	-2.163523	1.906911	0.000240
10	17	0	2.608060	-0.929266	0.000194
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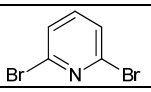
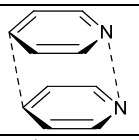
Ligand:	
Total electronic energy (in a.u.)	-5395.41136
Thermal Correction to Gibbs Free Energy (in a.u.)	0.034952

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000004	-0.332901	-0.000130
2	6	0	1.126940	0.362438	0.000155
3	6	0	1.204231	1.750208	0.000095
4	6	0	0.000012	2.448534	0.000035
5	1	0	-0.000014	3.537900	0.000133
6	6	0	-1.204231	1.750196	-0.000093
7	6	0	-1.126961	0.362448	-0.000386
8	1	0	-2.159827	2.268093	0.000001
9	1	0	2.159848	2.268067	0.000157
10	35	0	-2.740437	-0.654095	0.000053
11	35	0	2.740438	-0.654096	-0.000002

Complex:	
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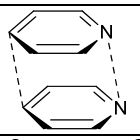
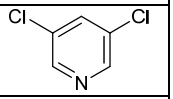
Total electronic energy (in a.u.)	-496.47037
Thermal Correction to Gibbs Free Energy (in a.u.)	0.138762

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.183083	-0.132203	-1.528014
2	6	0	1.433390	1.073021	-0.998831
3	1	0	1.104922	1.934879	-1.581363
4	6	0	2.079877	1.261905	0.220248
5	6	0	2.483879	0.140692	0.940431
6	1	0	2.990697	0.247179	1.899363
7	6	0	2.219684	-1.119691	0.410009
8	6	0	1.567749	-1.201700	-0.817759
9	1	0	1.347620	-2.176760	-1.254698
10	7	0	-2.570799	-0.234002	-0.919521
11	6	0	-2.110391	-1.249748	-0.176034
12	1	0	-2.327402	-2.254322	-0.541793
13	6	0	-1.390863	-1.078929	1.003929
14	6	0	-1.127213	0.216057	1.441986
15	1	0	-0.560845	0.391144	2.356248
16	6	0	-1.595404	1.282690	0.678506
17	6	0	-2.305769	1.007077	-0.486426
18	1	0	-2.681207	1.825010	-1.102938
19	1	0	-1.040914	-1.947849	1.559061
20	1	0	-1.409747	2.314714	0.972227
21	1	0	2.253678	2.269878	0.594152
22	1	0	2.507584	-2.028678	0.936116

Complex:	
Ligand:	
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Thermal Correction to Gibbs Free Energy (in a.u.)	0.094769

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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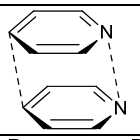
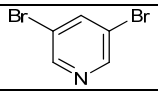
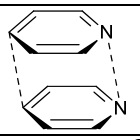
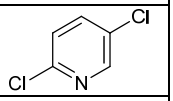
2	17	0	-0.658561	2.251438	-1.574569
3	7	0	1.019705	1.495875	1.946468
4	6	0	2.123849	0.829477	1.601084
5	1	0	2.780436	0.496785	2.403954
6	6	0	2.442766	0.567741	0.271922
7	6	0	1.611789	1.000478	-0.752281
8	1	0	1.843310	0.816605	-1.799164
9	6	0	0.462254	1.675697	-0.364696
10	6	0	0.190363	1.900340	0.981702
11	1	0	-0.712970	2.428765	1.283697
12	17	0	-3.917889	0.285830	-0.092292
13	17	0	0.630679	-2.362800	-1.457010
14	7	0	-0.965827	-1.319986	2.028803
15	6	0	-2.084752	-0.693675	1.656569
16	1	0	-2.723921	-0.297955	2.444806
17	6	0	-2.439877	-0.550941	0.318609
18	6	0	-1.630843	-1.063362	-0.686235
19	1	0	-1.891184	-0.970330	-1.738368
20	6	0	-0.465864	-1.694823	-0.272196
21	6	0	-0.157953	-1.800655	1.081071
22	1	0	0.757529	-2.294644	1.404039

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-10790.82386
Thermal Correction to Gibbs Free Energy (in a.u.)	0.088991

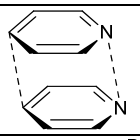
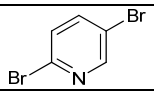
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	4.076331	0.187299	0.322640
2	35	0	-0.957575	2.229518	-1.418444
3	7	0	0.706078	1.516341	2.278402
4	6	0	1.914542	1.034016	1.979068
5	1	0	2.558326	0.760472	2.814139
6	6	0	2.349704	0.888918	0.664285
7	6	0	1.521993	1.250564	-0.391591
8	1	0	1.842493	1.158730	-1.427372
9	6	0	0.261537	1.730376	-0.056386
10	6	0	-0.115824	1.844623	1.279199
11	1	0	-1.101041	2.221454	1.551655
12	35	0	-4.076977	-0.193417	0.313901
13	35	0	0.965351	-2.189106	-1.457418
14	7	0	-0.720675	-1.586205	2.248824
15	6	0	-1.926293	-1.092692	1.956778
16	1	0	-2.574869	-0.842987	2.795609
17	6	0	-2.353186	-0.907337	0.644276
18	6	0	-1.519521	-1.238073	-0.416942
19	1	0	-1.833732	-1.115772	-1.451504
20	6	0	-0.261497	-1.729152	-0.088671
21	6	0	0.107122	-1.884862	1.245123
22	1	0	1.089963	-2.271428	1.512259

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2334.89384
Thermal Correction to Gibbs Free Energy (in a.u.)	0.093788

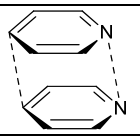
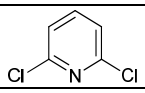
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.954621	2.333439	-0.611475
2	6	0	-1.901196	1.565691	-0.057453
3	1	0	-2.887086	1.585837	-0.517808
4	6	0	-1.645490	0.778635	1.058384
5	6	0	-0.380587	0.774245	1.636870
6	1	0	-0.160591	0.165741	2.511521
7	6	0	0.602381	1.566804	1.058949
8	6	0	0.244361	2.309824	-0.061084
9	17	0	1.470279	3.309348	-0.828279
10	7	0	0.450192	-0.846146	-1.650645
11	6	0	1.638545	-0.798949	-1.037365
12	1	0	2.405769	-0.174375	-1.492408
13	6	0	1.892415	-1.515962	0.124503
14	6	0	0.900237	-2.310194	0.689039
15	1	0	1.080141	-2.879417	1.599038
16	6	0	-0.335843	-2.353579	0.056469
17	6	0	-0.487331	-1.593193	-1.099798
18	17	0	-2.043028	-1.607210	-1.916009
19	17	0	3.464683	-1.393391	0.877993
20	1	0	-1.152627	-2.950891	0.453531
21	17	0	-2.923158	-0.208514	1.725538
22	1	0	1.611255	1.598186	1.462772

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-10790.83121
Thermal Correction to Gibbs Free Energy (in a.u.)	0.088843

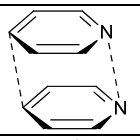
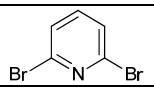
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.152496	2.559646	0.321761
2	6	0	1.272218	2.067814	-0.223083
3	1	0	2.214349	2.440211	0.176515
4	6	0	1.242172	1.134779	-1.253239
5	6	0	0.021643	0.689705	-1.751409
6	1	0	-0.035837	-0.040342	-2.556762
7	6	0	-1.140043	1.198940	-1.184640
8	6	0	-0.998828	2.119132	-0.149746
9	35	0	-2.575888	2.805224	0.676476
10	7	0	-0.095474	-0.794960	1.746175
11	6	0	-1.242031	-1.175395	1.170577
12	1	0	-2.159991	-0.774753	1.598627
13	6	0	-1.269240	-2.044172	0.085968
14	6	0	-0.079812	-2.546666	-0.431809
15	1	0	-0.067605	-3.229386	-1.279492
16	6	0	1.111213	-2.147711	0.162423
17	6	0	1.028070	-1.266285	1.237716
18	35	0	2.643363	-0.686270	2.067185
19	35	0	-2.935485	-2.515721	-0.685233
20	1	0	2.067068	-2.511292	-0.205816
21	35	0	2.868836	0.473897	-1.962631
22	1	0	-2.118234	0.882371	-1.538054

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2334.90106
Thermal Correction to Gibbs Free Energy (in a.u.)	0.094628

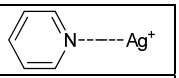
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.366527	-0.761765	-0.935374
2	6	0	-0.602682	-1.775123	-0.560695
3	17	0	0.696582	-2.202423	-1.658415
4	6	0	-0.762791	-2.507070	0.608949
5	6	0	-1.806755	-2.129805	1.447875
6	1	0	-1.979672	-2.665162	2.380110
7	6	0	-2.625160	-1.060462	1.094907
8	6	0	-2.342913	-0.425615	-0.107340
9	17	0	-3.338621	0.929270	-0.607522
10	7	0	1.768777	1.338817	-0.230445
11	6	0	0.648358	1.857486	0.245882
12	17	0	-0.018559	3.200074	-0.665041
13	6	0	-0.010463	1.423571	1.388995
14	6	0	0.557006	0.351614	2.070872
15	1	0	0.080160	-0.038211	2.968408
16	6	0	1.732709	-0.225396	1.598062
17	6	0	2.280386	0.322382	0.446367
18	17	0	3.775132	-0.344236	-0.186724
19	1	0	-0.928231	1.897623	1.726649
20	1	0	2.202228	-1.065609	2.102180
21	1	0	-0.097411	-3.330433	0.853956
22	1	0	-3.446054	-0.732720	1.727117

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-10790.83583
Thermal Correction to Gibbs Free Energy (in a.u.)	0.090401

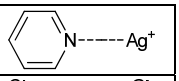
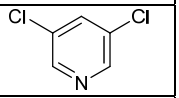
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.716401	1.697255	-0.560728
2	6	0	-0.328792	2.289847	-0.004617
3	35	0	-1.926684	2.317062	-1.040607
4	6	0	-0.330618	2.883352	1.252636
5	6	0	0.859214	2.838783	1.973033
6	1	0	0.914982	3.284936	2.964752
7	6	0	1.975429	2.214454	1.423800
8	6	0	1.829898	1.665810	0.155066
9	35	0	3.323911	0.804435	-0.653853
10	7	0	-0.798230	-1.993363	-0.028133
11	6	0	0.422888	-1.957459	0.483047
12	35	0	1.732929	-3.021267	-0.401708
13	6	0	0.791615	-1.225707	1.605685
14	6	0	-0.204736	-0.477270	2.225778
15	1	0	0.027794	0.117141	3.107596
16	6	0	-1.499132	-0.489696	1.713487
17	6	0	-1.723269	-1.272934	0.587512
18	35	0	-3.482532	-1.371755	-0.138763
19	1	0	1.810483	-1.239435	1.983809
20	1	0	-2.297814	0.084678	2.175594
21	1	0	-1.221411	3.356970	1.656715
22	1	0	2.916965	2.156739	1.963564

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-395.09382
Thermal Correction to Gibbs Free Energy (in a.u.)	0.058566

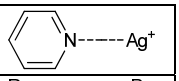
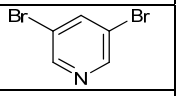
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.185648	-1.155333	0.000002
2	1	0	-0.598132	-2.071610	0.000003
3	6	0	-2.573758	-1.198379	-0.000001
4	6	0	-3.282838	0.000200	-0.000002
5	6	0	-2.573408	1.198578	-0.000001
6	6	0	-1.185312	1.155134	0.000002
7	7	0	-0.498155	-0.000210	0.000003
8	1	0	-3.082414	-2.160479	-0.000002
9	1	0	-4.372444	0.000358	-0.000004
10	1	0	-3.081793	2.160821	-0.000002
11	1	0	-0.597545	2.071248	0.000003
12	47	0	1.702664	-0.000002	-0.000001

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1314.29306
Thermal Correction to Gibbs Free Energy (in a.u.)	0.035014

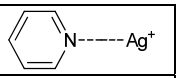
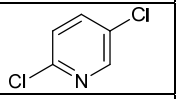
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	2.613958	-0.000156	0.000059
2	7	0	0.389994	-0.000226	-0.000290
3	6	0	-0.282743	-1.158212	-0.000221
4	6	0	-1.671856	-1.181066	-0.000079
5	6	0	-2.401817	0.000216	0.000005
6	1	0	-3.490227	0.000390	0.000140
7	6	0	-1.671482	1.181271	-0.000071
8	6	0	-0.282380	1.157982	-0.000223
9	17	0	-2.494588	2.717713	0.000094
10	17	0	-2.495432	-2.717255	0.000095
11	1	0	0.298452	2.077294	-0.000274
12	1	0	0.297807	-2.077701	-0.000275

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5542.26206
Thermal Correction to Gibbs Free Energy (in a.u.)	0.031653

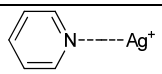
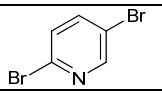
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	3.219292	-0.000587	0.000216
2	7	0	0.992829	-0.000369	-0.001095
3	6	0	0.319861	-1.158175	-0.000763
4	6	0	-1.069873	-1.184372	-0.000107
5	6	0	-1.796872	0.000384	0.000246
6	1	0	-2.885496	0.000558	0.000743
7	6	0	-1.069273	1.184739	-0.000118
8	6	0	0.320465	1.157765	-0.000793
9	1	0	0.909255	2.072510	-0.001263
10	1	0	0.908183	-2.073231	-0.001159
11	35	0	-1.962332	2.852533	0.000123
12	35	0	-1.963792	-2.851725	0.000118

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1314.29609
Thermal Correction to Gibbs Free Energy (in a.u.)	0.034170

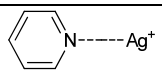
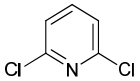
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	1.998000	-0.951205	-0.000492
2	7	0	-0.017298	0.041023	0.001949
3	6	0	-1.124531	-0.718925	0.001911
4	6	0	-2.389047	-0.150320	0.000132
5	6	0	-2.537182	1.232624	-0.001616
6	1	0	-3.521917	1.696080	-0.002982
7	6	0	-1.389154	2.013740	-0.001435
8	6	0	-0.162443	1.363127	0.000401
9	17	0	-3.786987	-1.191901	0.000070
10	1	0	-0.984035	-1.797193	0.003396
11	1	0	-1.446021	3.098966	-0.002688
12	17	0	1.303528	2.308380	0.000835

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5542.26296
Thermal Correction to Gibbs Free Energy (in a.u.)	0.030659

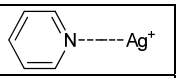
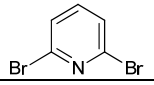
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-1.847028	-1.715335	-0.000044
2	7	0	-0.242660	-0.145303	0.000144
3	6	0	1.036960	-0.554354	0.000101
4	6	0	2.089125	0.350333	-0.000015
5	6	0	1.830295	1.717209	-0.000182
6	1	0	2.633230	2.452398	-0.000333
7	6	0	0.505567	2.136712	-0.000171
8	6	0	-0.486167	1.164221	0.000047
9	1	0	1.204321	-1.629065	0.000195
10	1	0	0.260621	3.195711	-0.000322
11	35	0	3.864983	-0.300833	0.000027
12	35	0	-2.306237	1.693235	0.000054

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1314.29824
Thermal Correction to Gibbs Free Energy (in a.u.)	0.033843

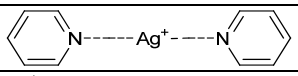
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	1.825176	-0.002134	0.000436
2	7	0	-0.464997	-0.000293	-0.000299
3	6	0	-1.166852	-1.135448	0.000049
4	6	0	-2.550914	-1.199946	0.000573
5	6	0	-3.245947	0.005035	0.000955
6	1	0	-4.334743	0.007039	0.001216
7	6	0	-2.546262	1.207423	0.000654
8	6	0	-1.162483	1.137826	-0.000034
9	1	0	-3.056385	2.166574	0.000682
10	1	0	-3.064782	-2.157095	0.000506
11	17	0	-0.232032	2.613124	-0.001004
12	17	0	-0.240771	-2.613331	-0.000994

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5542.26245
Thermal Correction to Gibbs Free Energy (in a.u.)	0.031659

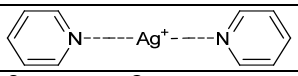
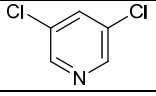
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.002426	-1.830938	-0.000031
2	7	0	0.000803	0.445039	0.000147
3	6	0	1.141304	1.141817	0.000067
4	6	0	1.206320	2.526345	-0.000034
5	6	0	0.002818	3.224441	-0.000082
6	1	0	0.003618	4.313251	-0.000179
7	6	0	-1.201753	2.528075	-0.000048
8	6	0	-1.138759	1.143498	0.000081
9	1	0	-2.154582	3.050125	-0.000125
10	1	0	2.159957	3.046916	-0.000089
11	35	0	-2.742919	0.132489	0.000014
12	35	0	2.744058	0.128753	0.000013

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-643.36238
Thermal Correction to Gibbs Free Energy (in a.u.)	0.139498

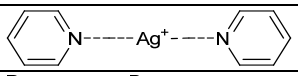
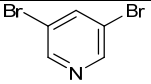
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.820934	-1.141150	-0.186446
2	1	0	-2.233096	-2.044858	-0.334248
3	6	0	-4.208410	-1.182789	-0.193846
4	6	0	-4.917884	-0.000283	-0.000640
5	6	0	-4.208839	1.182394	0.193064
6	6	0	-2.821344	1.141106	0.186600
7	7	0	-2.133550	0.000070	0.000303
8	1	0	-4.716534	-2.132416	-0.349704
9	1	0	-6.007372	-0.000418	-0.001018
10	1	0	-4.717299	2.131892	0.348605
11	1	0	-2.233828	2.044947	0.334867
12	47	0	-0.000001	0.000169	0.000297
13	7	0	2.133553	0.000128	0.000241
14	6	0	2.821250	1.141155	-0.186479
15	6	0	4.208741	1.182417	-0.193815
16	6	0	4.917885	-0.000278	-0.000575
17	6	0	4.208512	-1.182767	0.193092
18	6	0	2.821030	-1.141100	0.186570
19	1	0	2.233658	2.045015	-0.334322
20	1	0	4.717125	2.131908	-0.349655
21	1	0	6.007373	-0.000435	-0.000899
22	1	0	4.716712	-2.132401	0.348648
23	1	0	2.233267	-2.044786	0.334806

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2481.75989
Thermal Correction to Gibbs Free Energy (in a.u.)	0.093309

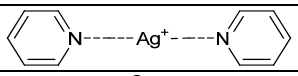
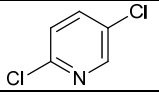
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.000002	-0.000052	0.000150
2	7	0	-2.155280	-0.000013	0.000272
3	6	0	-2.827779	1.134597	0.238242
4	6	0	-4.216425	1.156237	0.243082
5	17	0	-5.039892	2.658674	0.560126
6	6	0	-4.945852	0.000003	-0.000151
7	1	0	-6.034091	0.000012	-0.000303
8	6	0	-4.216367	-1.156241	-0.243156
9	17	0	-5.039775	-2.658666	-0.560407
10	6	0	-2.827721	-1.134619	-0.237894
11	7	0	2.155279	-0.000017	-0.000086
12	6	0	2.827722	1.134610	-0.238143
13	6	0	4.216368	1.156276	-0.243180
14	17	0	5.039768	2.658726	-0.560336
15	6	0	4.945849	0.000054	-0.000050
16	1	0	6.034089	0.000085	-0.000046
17	6	0	4.216421	-1.156204	0.243054
18	17	0	5.039899	-2.658614	0.560200
19	6	0	2.827774	-1.134609	0.237984
20	1	0	2.246520	2.033854	-0.427144
21	1	0	2.246618	-2.033891	0.426948
22	1	0	-2.246523	-2.033892	-0.426771
23	1	0	-2.246624	2.033850	0.427343

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-10937.69791
Thermal Correction to Gibbs Free Energy (in a.u.)	0.088013

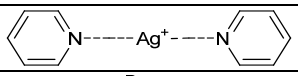
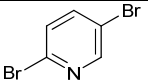
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.000003	-0.000143	0.000103
2	7	0	-2.157476	-0.000059	0.000842
3	6	0	-2.830293	1.126200	0.274367
4	6	0	-4.219555	1.151166	0.280857
5	6	0	-4.946312	0.000026	-0.000096
6	1	0	-6.034961	0.000056	-0.000441
7	6	0	-4.219442	-1.151175	-0.280549
8	6	0	-2.830199	-1.126294	-0.273113
9	7	0	2.157473	-0.000109	-0.000749
10	6	0	2.830229	1.126183	-0.274304
11	6	0	4.219489	1.151204	-0.280877
12	6	0	4.946304	0.000090	0.000038
13	1	0	6.034954	0.000170	0.000311
14	6	0	4.219498	-1.151141	0.280534
15	6	0	2.830254	-1.126313	0.273177
16	1	0	2.241528	2.014616	-0.490055
17	1	0	2.241553	-2.014857	0.488465
18	1	0	-2.241457	-2.014815	-0.488376
19	1	0	-2.241636	2.014658	0.490145
20	35	0	-5.111412	-2.771010	-0.677988
21	35	0	-5.111649	2.771067	0.677665
22	35	0	5.111536	-2.770944	0.677906
23	35	0	5.111535	2.771127	-0.677748

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2481.76521
Thermal Correction to Gibbs Free Energy (in a.u.)	0.092113

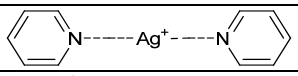
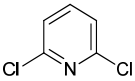
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.000010	0.077456	0.000163
2	7	0	-2.177125	0.053394	0.086739
3	6	0	-2.901916	1.109702	0.452239
4	6	0	-4.288569	1.114081	0.518925
5	6	0	-4.960413	-0.054336	0.185838
6	1	0	-6.047200	-0.097096	0.224949
7	6	0	-4.206041	-1.158611	-0.195448
8	6	0	-2.823119	-1.080223	-0.237119
9	7	0	2.177130	0.053436	-0.086685
10	6	0	2.901883	1.109714	-0.452335
11	6	0	4.288529	1.114078	-0.519193
12	6	0	4.960402	-0.054323	-0.186112
13	1	0	6.047184	-0.097095	-0.225353
14	6	0	4.206067	-1.158569	0.195336
15	6	0	2.823151	-1.080170	0.237166
16	1	0	-4.829538	2.006026	0.823803
17	1	0	-2.212356	-1.930159	-0.531846
18	17	0	-2.022255	2.555014	0.866094
19	17	0	-4.982067	-2.658387	-0.626761
20	1	0	2.212418	-1.930083	0.532019
21	1	0	4.829465	2.006000	-0.824196
22	17	0	2.022167	2.554996	-0.866175
23	17	0	4.982136	-2.658322	0.626655

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-10937.70093
Thermal Correction to Gibbs Free Energy (in a.u.)	0.087011

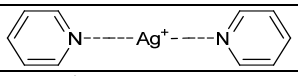
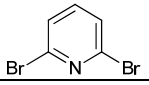
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.000005	0.088467	-0.000037
2	7	0	-2.173198	0.081113	0.136798
3	6	0	-2.904846	1.141840	0.482462
4	6	0	-4.291284	1.129260	0.559473
5	6	0	-4.953375	-0.054935	0.259116
6	1	0	-6.040007	-0.098385	0.310454
7	6	0	-4.193015	-1.162114	-0.102962
8	6	0	-2.810432	-1.066376	-0.154802
9	7	0	2.173176	0.081037	-0.137107
10	6	0	2.904919	1.141795	-0.482472
11	6	0	4.291371	1.129191	-0.559218
12	6	0	4.953376	-0.055046	-0.258854
13	1	0	6.040016	-0.098520	-0.309978
14	6	0	4.192923	-1.162249	0.102955
15	6	0	2.810329	-1.066502	0.154491
16	1	0	-4.848374	2.017696	0.845683
17	1	0	-2.185247	-1.911666	-0.432269
18	1	0	2.185072	-1.911827	0.431692
19	1	0	4.848530	2.017647	-0.845234
20	35	0	-5.018503	-2.808954	-0.530296
21	35	0	-1.964713	2.735345	0.883043
22	35	0	1.964916	2.735385	-0.883015
23	35	0	5.018318	-2.809122	0.530337

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2481.76896
Thermal Correction to Gibbs Free Energy (in a.u.)	0.092270

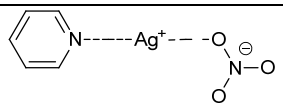
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.000008	0.031512	0.000063
2	7	0	-2.207329	0.000642	-0.007411
3	6	0	-2.922335	1.070614	0.353913
4	6	0	-4.306527	1.111987	0.375522
5	6	0	-4.986864	-0.041214	-0.002011
6	1	0	-6.075478	-0.057792	0.000262
7	6	0	-4.273429	-1.173138	-0.382742
8	6	0	-2.890958	-1.090514	-0.366684
9	7	0	2.207334	0.000637	0.007358
10	6	0	2.922548	1.070475	-0.353939
11	6	0	4.306752	1.111597	-0.375446
12	6	0	4.986867	-0.041713	0.002154
13	1	0	6.075477	-0.058472	-0.000036
14	6	0	4.273208	-1.173514	0.382834
15	6	0	2.890755	-1.090642	0.366663
16	1	0	-4.772106	-2.090319	-0.683563
17	1	0	-4.831347	2.013970	0.678002
18	1	0	4.831756	2.013481	-0.677908
19	1	0	4.771684	-2.090789	0.683703
20	17	0	-1.940579	-2.471304	-0.837727
21	17	0	-2.010978	2.478838	0.820600
22	17	0	1.940106	-2.471293	0.837591
23	17	0	2.011467	2.478835	-0.820736

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-10937.70105
Thermal Correction to Gibbs Free Energy (in a.u.)	0.089008

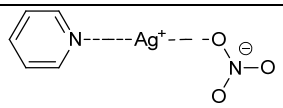
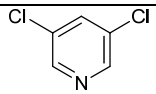
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.000000	-0.000001	0.000001
2	7	0	-2.199238	-0.000002	0.000001
3	6	0	-2.896883	1.049385	0.452370
4	6	0	-4.280983	1.106128	0.475896
5	6	0	-4.977927	-0.000002	0.000003
6	1	0	-6.066684	-0.000002	0.000005
7	6	0	-4.280984	-1.106131	-0.475892
8	6	0	-2.896884	-1.049387	-0.452369
9	7	0	2.199238	0.000000	-0.000001
10	6	0	2.896886	-1.049384	0.452368
11	6	0	4.280986	-1.106123	0.475892
12	6	0	4.977927	0.000008	-0.000002
13	1	0	6.066684	0.000011	-0.000002
14	6	0	4.280980	1.106136	-0.475896
15	6	0	2.896880	1.049388	-0.452371
16	1	0	-4.801727	-1.982433	-0.852155
17	1	0	-4.801727	1.982430	0.852160
18	1	0	4.801733	-1.982423	0.852155
19	1	0	4.801721	1.982439	-0.852160
20	35	0	-1.884157	-2.517689	-1.086208
21	35	0	-1.884156	2.517687	1.086208
22	35	0	1.884163	-2.517688	1.086208
23	35	0	1.884150	2.517688	-1.086208

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-675.54034
Thermal Correction to Gibbs Free Energy (in a.u.)	0.065226

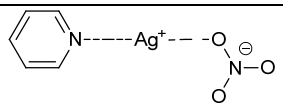
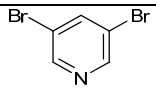
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.489278	0.312960	0.082760
2	8	0	-2.630249	0.728839	0.162116
3	8	0	-4.597748	-0.125728	-0.066472
4	7	0	1.636123	0.036964	0.021788
5	7	0	-3.371345	-0.279155	-0.086014
6	6	0	2.468597	1.078317	-0.155684
7	6	0	3.847695	0.928725	-0.214536
8	1	0	4.477092	1.804469	-0.360352
9	6	0	4.392365	-0.346287	-0.085216
10	1	0	5.470615	-0.496646	-0.127777
11	6	0	3.532649	-1.426135	0.099000
12	1	0	3.908770	-2.441833	0.204983
13	6	0	2.164873	-1.193683	0.146649
14	8	0	-2.849647	-1.374585	-0.337297
15	1	0	1.462531	-2.012754	0.288272
16	1	0	2.007675	2.059181	-0.253332

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1594.73932
Thermal Correction to Gibbs Free Energy (in a.u.)	0.040643

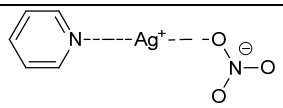
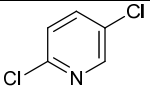
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	1.450336	0.402033	-0.000156
2	8	0	3.598904	0.803201	-0.000435
3	8	0	5.546339	-0.125510	-0.000013
4	7	0	-0.696044	0.129950	0.000056
5	7	0	4.316905	-0.250853	0.000160
6	6	0	-1.524046	1.183394	0.000122
7	6	0	-2.902393	1.010465	0.000100
8	17	0	-3.932847	2.415811	0.000177
9	6	0	-3.460113	-0.261147	0.000017
10	1	0	-4.537631	-0.413496	-0.000010
11	6	0	-2.572267	-1.328705	-0.000033
12	17	0	-3.170491	-2.965505	-0.000121
13	6	0	-1.200578	-1.111738	-0.000018
14	8	0	3.768923	-1.362518	0.000901
15	1	0	-0.496783	-1.940579	-0.000069
16	1	0	-1.077617	2.174625	0.000192

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5822.70829
Thermal Correction to Gibbs Free Energy (in a.u.)	0.038219

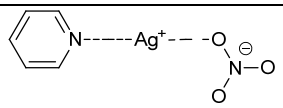
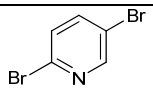
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-2.171747	0.121401	-0.339149
2	8	0	-4.460442	-0.328949	1.438804
3	8	0	-6.260950	-0.000562	0.282171
4	7	0	-0.014419	0.046052	-0.164357
5	7	0	-5.029357	-0.039413	0.376917
6	6	0	0.613638	-1.136913	-0.119676
7	6	0	1.995574	-1.214406	0.003705
8	6	0	2.761921	-0.057600	0.083939
9	1	0	3.845220	-0.097796	0.182748
10	6	0	2.081296	1.153200	0.033173
11	6	0	0.697457	1.178911	-0.090218
12	8	0	-4.332503	0.228846	-0.657432
13	1	0	0.144214	2.114177	-0.129798
14	1	0	-0.005342	-2.028696	-0.184476
15	35	0	3.031164	2.786254	0.129871
16	35	0	2.823872	-2.914078	0.058978

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1594.74210
Thermal Correction to Gibbs Free Energy (in a.u.)	0.040576

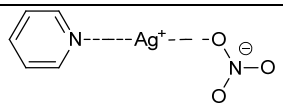
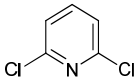
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-1.097003	-0.344236	-0.216178
2	8	0	-3.593206	0.306594	1.114347
3	8	0	-5.190792	-0.781039	0.137184
4	7	0	1.019971	0.167836	-0.053071
5	7	0	-3.996716	-0.483238	0.248325
6	6	0	1.920012	-0.828718	0.006985
7	6	0	3.278387	-0.569662	0.100033
8	6	0	3.742050	0.741093	0.134603
9	1	0	4.804744	0.964708	0.207840
10	6	0	2.808546	1.766926	0.072582
11	6	0	1.466874	1.421933	-0.020299
12	8	0	-3.160164	-1.010315	-0.557051
13	1	0	1.534254	-1.844712	-0.021398
14	17	0	4.391973	-1.908970	0.172943
15	1	0	3.115597	2.809151	0.096402
16	17	0	0.266842	2.682289	-0.102857

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5822.70958
Thermal Correction to Gibbs Free Energy (in a.u.)	0.036865

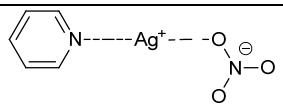
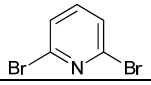
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-1.527294	-0.457823	-0.325306
2	8	0	-3.614481	-1.388843	1.416938
3	8	0	-5.321045	-1.972987	0.218055
4	7	0	0.522778	0.271224	-0.091399
5	7	0	-4.172564	-1.529814	0.318753
6	6	0	1.509769	-0.641868	-0.090794
7	6	0	2.839075	-0.274626	0.058479
8	6	0	3.177201	1.065716	0.212956
9	1	0	4.210911	1.385149	0.332687
10	6	0	2.154929	2.006662	0.211609
11	6	0	0.850533	1.555416	0.056524
12	8	0	-3.546648	-1.208867	-0.745381
13	1	0	1.211297	-1.680289	-0.213762
14	1	0	2.376140	3.064465	0.329443
15	35	0	4.172857	-1.615644	0.049228
16	35	0	-0.567106	2.811537	0.049058

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1594.74409
Thermal Correction to Gibbs Free Energy (in a.u.)	0.039818

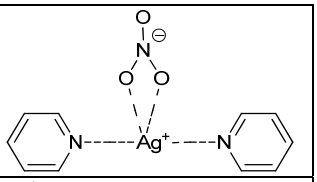
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.799297	-0.345177	-0.076179
2	8	0	3.197747	1.198728	0.378208
3	8	0	4.920025	-0.075886	0.062394
4	7	0	-1.371531	0.056514	-0.012240
5	7	0	3.697155	0.100952	0.090825
6	6	0	-1.850898	1.303816	-0.016353
7	6	0	-3.198148	1.621632	0.036643
8	6	0	-4.102344	0.566360	0.099493
9	1	0	-5.171639	0.766266	0.144218
10	6	0	-3.637089	-0.744768	0.103944
11	6	0	-2.266109	-0.934366	0.045150
12	8	0	2.932759	-0.881299	-0.185752
13	17	0	-1.619989	-2.551788	0.040688
14	17	0	-0.668950	2.580134	-0.096376
15	1	0	-4.314182	-1.593162	0.150912
16	1	0	-3.525248	2.657682	0.029833

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5822.70966
Thermal Correction to Gibbs Free Energy (in a.u.)	0.037433

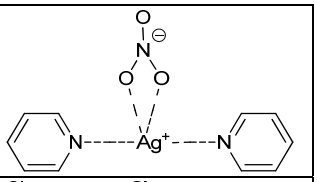
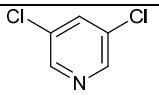
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.977193	-0.336278	-0.221820
2	8	0	3.405052	0.402072	1.107337
3	8	0	5.071402	-0.586787	0.139580
4	7	0	-1.168415	0.165760	-0.004831
5	7	0	3.862437	-0.356132	0.239480
6	6	0	-1.579333	1.439479	0.026395
7	6	0	-2.905841	1.826068	0.134995
8	6	0	-3.863669	0.821253	0.221944
9	1	0	-4.918232	1.077462	0.309244
10	6	0	-3.468929	-0.512234	0.199304
11	6	0	-2.113426	-0.778191	0.084160
12	8	0	3.063549	-0.919887	-0.580487
13	1	0	-4.195241	-1.317345	0.270055
14	1	0	-3.185661	2.875734	0.153247
15	35	0	-1.519463	-2.575307	0.046854
16	35	0	-0.229678	2.762747	-0.083476

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-923.79204
Thermal Correction to Gibbs Free Energy (in a.u.)	0.144933

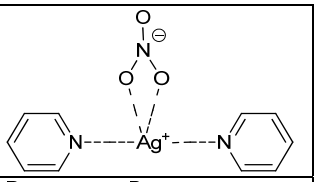
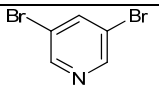
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.028193	-0.726363	-0.038512
2	8	0	-0.016362	2.443434	-1.023982
3	8	0	0.168439	4.266904	0.127988
4	7	0	-2.166419	-0.695169	-0.019270
5	7	0	0.118568	3.019546	0.077924
6	6	0	-2.884911	-1.827221	-0.123309
7	6	0	-4.273123	-1.833035	-0.108133
8	1	0	-4.807609	-2.776853	-0.195939
9	6	0	-4.949402	-0.622449	0.020487
10	1	0	-6.038409	-0.594123	0.036418
11	6	0	-4.207506	0.550817	0.129231
12	1	0	-4.688682	1.521315	0.232747
13	6	0	-2.821765	0.472617	0.104652
14	8	0	0.203478	2.347888	1.128993
15	7	0	2.110094	-0.757859	-0.036334
16	6	0	2.792821	-1.865476	0.304113
17	6	0	4.180105	-1.905294	0.337442
18	1	0	4.684777	-2.827055	0.620243
19	6	0	4.893847	-0.756271	0.006480
20	1	0	5.983223	-0.755676	0.023380
21	6	0	4.189114	0.391196	-0.347575
22	1	0	4.701002	1.313233	-0.615913
23	6	0	2.801412	0.350225	-0.356766
24	1	0	2.201625	-2.743351	0.556926
25	1	0	2.215901	1.225184	-0.633673
26	1	0	-2.208151	1.367601	0.187979
27	1	0	-2.322291	-2.753307	-0.222073

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2762.19091
Thermal Correction to Gibbs Free Energy (in a.u.)	0.097581

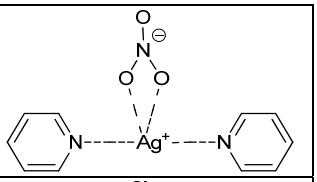
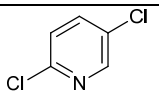
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.003352	-0.246602	-0.018342
2	8	0	0.057827	2.542436	1.018330
3	8	0	-0.072255	4.270231	-0.280962
4	7	0	2.177285	-0.421746	0.012407
5	7	0	-0.020440	3.033255	-0.129180
6	6	0	2.771533	-1.592446	0.277839
7	6	0	4.155776	-1.704831	0.305388
8	17	0	4.872873	-3.254507	0.657277
9	6	0	4.963050	-0.602650	0.056499
10	1	0	6.048878	-0.672173	0.073751
11	6	0	4.313051	0.593908	-0.215145
12	17	0	5.236608	2.035450	-0.542609
13	6	0	2.925942	0.661543	-0.231334
14	8	0	-0.046993	2.278327	-1.128147
15	7	0	-2.170332	-0.425347	0.011946
16	6	0	-2.771452	-1.579938	-0.303814
17	6	0	-4.156018	-1.691432	-0.304724
18	17	0	-4.883113	-3.218648	-0.726905
19	6	0	-4.956419	-0.605712	0.024817
20	1	0	-6.042385	-0.675466	0.029468
21	6	0	-4.299446	0.574226	0.347676
22	17	0	-5.214253	1.994043	0.778309
23	6	0	-2.912300	0.642285	0.333349
24	1	0	-2.135892	-2.424330	-0.558694
25	1	0	-2.387488	1.560703	0.587300
26	1	0	2.406145	1.592303	-0.446380
27	1	0	2.130713	-2.449272	0.470147

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-11218.12935
Thermal Correction to Gibbs Free Energy (in a.u.)	0.092145

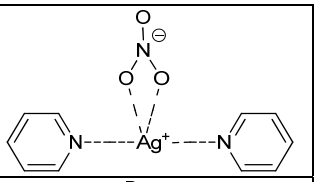
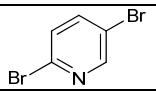
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.001787	0.119507	-0.017503
2	8	0	-0.052300	-2.678213	0.999549
3	8	0	0.056658	-4.397207	-0.313450
4	7	0	-2.179130	0.290045	-0.004372
5	7	0	0.015281	-3.161263	-0.152093
6	6	0	-2.784903	1.459696	0.238400
7	6	0	-4.170730	1.561395	0.266791
8	6	0	-4.964836	0.442410	0.043063
9	1	0	-6.051662	0.502178	0.062410
10	6	0	-4.306172	-0.755919	-0.205942
11	6	0	-2.917726	-0.804844	-0.225060
12	8	0	0.041530	-2.398566	-1.145388
13	7	0	2.174933	0.290167	0.027344
14	6	0	2.783386	1.452408	-0.242793
15	6	0	4.169344	1.554539	-0.256328
16	6	0	4.960703	0.443572	0.011615
17	1	0	6.047657	0.503463	0.004501
18	6	0	4.299436	-0.747118	0.288998
19	6	0	2.910840	-0.797116	0.291277
20	1	0	2.145646	2.308342	-0.450438
21	1	0	2.373014	-1.716567	0.512013
22	1	0	-2.381373	-1.729661	-0.423738
23	1	0	-2.145207	2.321892	0.411220
24	35	0	-5.289323	-2.341362	-0.521965
25	35	0	-4.965625	3.242571	0.615348
26	35	0	4.968444	3.225004	-0.644627
27	35	0	5.280080	-2.320537	0.666235

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2762.19764
Thermal Correction to Gibbs Free Energy (in a.u.)	0.097433

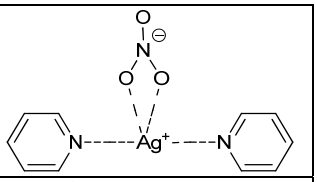
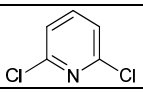
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.000009	-0.265045	0.000480
2	8	0	-0.064871	2.251081	-1.081198
3	8	0	-0.001361	4.127005	-0.001190
4	7	0	-2.204098	-0.484222	-0.099994
5	7	0	-0.000424	2.881861	-0.001046
6	6	0	-2.830692	-1.576141	-0.529470
7	6	0	-4.211335	-1.694793	-0.626457
8	6	0	-4.985216	-0.603980	-0.253636
9	1	0	-6.070995	-0.649032	-0.313872
10	6	0	-4.332537	0.539182	0.195296
11	6	0	-2.948777	0.573364	0.261927
12	8	0	0.064976	2.251530	1.079475
13	7	0	2.204265	-0.484165	0.099980
14	6	0	2.830961	-1.576197	0.529076
15	6	0	4.211578	-1.694793	0.626133
16	6	0	4.985415	-0.603730	0.253875
17	1	0	6.071189	-0.648721	0.314219
18	6	0	4.332653	0.539518	-0.194640
19	6	0	2.948866	0.573602	-0.261478
20	1	0	-4.669239	-2.612955	-0.984757
21	1	0	-2.415802	1.454200	0.613979
22	17	0	-1.826003	-2.923645	-0.992350
23	17	0	-5.240315	1.946559	0.681141
24	1	0	2.416093	1.454587	-0.613534
25	1	0	4.669518	-2.613081	0.984063
26	17	0	1.826280	-2.923960	0.991304
27	17	0	5.240343	1.947206	-0.679842

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-11218.13424
Thermal Correction to Gibbs Free Energy (in a.u.)	0.091090

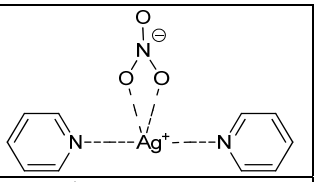
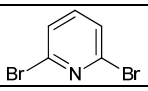
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.007751	0.161618	0.010146
2	8	0	-0.019631	-2.446699	-0.908373
3	8	0	-0.106975	-4.206393	0.351691
4	7	0	2.202734	0.383234	-0.216389
5	7	0	-0.037178	-2.969483	0.229368
6	6	0	2.817984	1.454338	-0.714283
7	6	0	4.195459	1.552410	-0.868550
8	6	0	4.974712	0.468473	-0.482853
9	1	0	6.057125	0.510612	-0.590108
10	6	0	4.334304	-0.652414	0.035785
11	6	0	2.952788	-0.666589	0.157122
12	8	0	0.015973	-2.237938	1.245277
13	7	0	-2.193560	0.381436	0.171300
14	6	0	-2.823275	1.427705	0.702552
15	6	0	-4.204169	1.515986	0.830011
16	6	0	-4.971129	0.447725	0.381357
17	1	0	-6.055786	0.482437	0.466509
18	6	0	-4.315472	-0.648566	-0.169638
19	6	0	-2.931741	-0.653441	-0.263249
20	1	0	4.656061	2.447206	-1.279298
21	1	0	2.418281	-1.523417	0.562420
22	1	0	-2.385385	-1.490426	-0.694398
23	1	0	-4.676708	2.391019	1.268722
24	35	0	5.324053	-2.169833	0.581003
25	35	0	1.718219	2.907119	-1.232615
26	35	0	-1.739772	2.857243	1.312232
27	35	0	-5.287459	-2.146681	-0.793733

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-2762.20094
Thermal Correction to Gibbs Free Energy (in a.u.)	0.095968

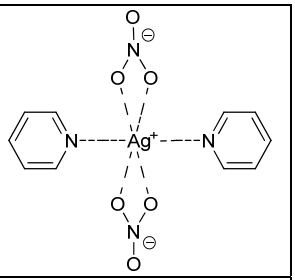
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.100695	0.316659	-0.125284
2	8	0	0.147722	2.401324	-1.465141
3	8	0	0.647405	4.397066	-0.786262
4	7	0	-2.219502	-0.580239	0.003072
5	7	0	0.443888	3.197902	-0.538149
6	6	0	-2.433676	-1.884967	-0.171562
7	6	0	-3.677501	-2.492292	-0.099057
8	6	0	-4.770478	-1.676297	0.175160
9	1	0	-5.768854	-2.105283	0.243080
10	6	0	-4.583973	-0.310442	0.361535
11	6	0	-3.288693	0.173400	0.262242
12	8	0	0.528544	2.762363	0.631872
13	7	0	2.085260	-0.475662	0.175386
14	6	0	2.637291	-0.554279	1.384039
15	6	0	3.943966	-0.949509	1.625733
16	6	0	4.720206	-1.285802	0.520840
17	1	0	5.753515	-1.601263	0.655889
18	6	0	4.172648	-1.220781	-0.756865
19	6	0	2.852684	-0.809606	-0.859656
20	1	0	-5.413527	0.357475	0.576026
21	1	0	-3.785460	-3.562529	-0.251489
22	1	0	4.336912	-0.992297	2.637810
23	1	0	4.748305	-1.479695	-1.641281
24	17	0	-2.992508	1.877348	0.484300
25	17	0	-1.026633	-2.857698	-0.513408
26	17	0	1.605007	-0.127241	2.725326
27	17	0	2.100608	-0.710996	-2.432220

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-11218.13676
Thermal Correction to Gibbs Free Energy (in a.u.)	0.088785

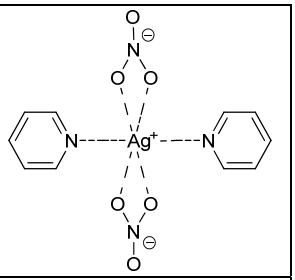
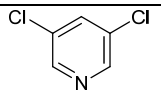
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.092686	-1.037413	-0.290512
2	8	0	0.274220	-3.239595	-0.978654
3	8	0	0.693287	-5.122804	0.000886
4	7	0	1.406646	0.838876	-0.956838
5	7	0	0.525117	-3.898131	0.073530
6	6	0	0.882336	1.992005	-1.368737
7	6	0	1.555143	3.205981	-1.354727
8	6	0	2.865723	3.204912	-0.887851
9	1	0	3.435230	4.132306	-0.857218
10	6	0	3.448014	2.013804	-0.463863
11	6	0	2.665696	0.870291	-0.520150
12	8	0	0.598948	-3.293901	1.160630
13	7	0	-1.545064	0.180136	0.968226
14	6	0	-1.221594	1.180995	1.785400
15	6	0	-2.094673	2.188558	2.171945
16	6	0	-3.393782	2.133159	1.677180
17	1	0	-4.115379	2.901171	1.950533
18	6	0	-3.768944	1.090694	0.834584
19	6	0	-2.798551	0.152424	0.516907
20	1	0	4.471233	1.982469	-0.099543
21	1	0	1.077208	4.119691	-1.697727
22	1	0	-1.776285	2.987540	2.836028
23	1	0	-4.778384	1.018389	0.438871
24	35	0	3.382219	-0.786423	0.067249
25	35	0	-0.897199	1.929393	-2.026022
26	35	0	0.553760	1.189091	2.459018
27	35	0	-3.231482	-1.279943	-0.652197

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1204.22321
Thermal Correction to Gibbs Free Energy (in a.u.)	0.151615

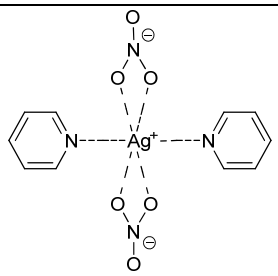
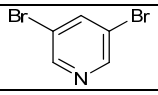
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.095414	-0.161941	-0.787994
2	8	0	-0.790036	1.777220	1.853284
3	8	0	-1.026356	2.909042	0.022551
4	8	0	-2.743295	2.517343	1.281912
5	8	0	1.396189	-2.597654	0.911400
6	8	0	1.145128	-0.929975	2.269512
7	8	0	3.132697	-1.585687	1.717073
8	7	0	1.980956	0.327376	-0.823188
9	7	0	-2.166957	-0.636600	-0.608387
10	7	0	-1.519387	2.403759	1.055433
11	7	0	1.891771	-1.706497	1.636236
12	6	0	2.443851	1.308468	-0.028627
13	1	0	1.698061	1.884786	0.516045
14	6	0	3.798116	1.585834	0.099154
15	6	0	4.712577	0.816843	-0.615669
16	1	0	5.781848	1.009414	-0.535395
17	6	0	4.235506	-0.204928	-1.432464
18	6	0	2.865928	-0.420113	-1.505342
19	1	0	2.455528	-1.211193	-2.129633
20	6	0	-3.113869	0.215165	-1.038617
21	1	0	-2.767195	1.105902	-1.558657
22	6	0	-4.468688	-0.015837	-0.840810
23	6	0	-4.862633	-1.170266	-0.170034
24	1	0	-5.917978	-1.379629	0.001124
25	6	0	-3.882852	-2.052568	0.279390
26	6	0	-2.549144	-1.749446	0.043599
27	1	0	-1.753320	-2.410056	0.383201
28	1	0	4.121610	2.392244	0.754184
29	1	0	4.910258	-0.836254	-2.007145
30	1	0	-5.195892	0.705356	-1.208351
31	1	0	-4.140532	-2.966855	0.810357

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-3042.62219
Thermal Correction to Gibbs Free Energy (in a.u.)	0.103556

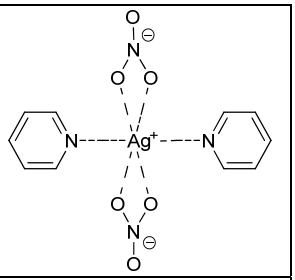
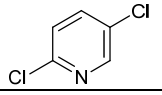
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.171823	0.087873	-0.650874
2	17	0	4.883769	2.238245	0.954539
3	17	0	4.859103	-2.538314	-1.640719
4	17	0	-5.640083	1.816961	-0.642310
5	17	0	-4.591635	-3.345811	0.702490
6	8	0	-0.506876	2.323072	1.249669
7	8	0	-0.352084	2.813437	-0.853829
8	8	0	-0.817071	4.361288	0.586483
9	8	0	0.729929	-2.402186	1.371306
10	8	0	0.910882	-0.538710	2.459383
11	8	0	2.664282	-1.755890	2.098242
12	7	0	2.015963	0.052996	-0.690007
13	7	0	-2.307817	-0.318481	-0.448191
14	7	0	-0.559121	3.167441	0.330543
15	7	0	1.434448	-1.567097	1.980319
16	6	0	2.686502	1.021094	-0.053170
17	1	0	2.112957	1.864874	0.323988
18	6	0	4.062884	0.947721	0.117554
19	6	0	4.781469	-0.138752	-0.363465
20	1	0	5.859448	-0.214466	-0.235477
21	6	0	4.052739	-1.126668	-1.011596
22	6	0	2.676209	-1.013176	-1.159193
23	1	0	2.095564	-1.784175	-1.659502
24	6	0	-3.185760	0.677656	-0.620684
25	1	0	-2.795247	1.639972	-0.944748
26	6	0	-4.542933	0.484292	-0.398142
27	6	0	-5.026328	-0.750362	0.014704
28	1	0	-6.086160	-0.918461	0.195955
29	6	0	-4.087078	-1.758962	0.185027
30	6	0	-2.738376	-1.522098	-0.049529
31	1	0	-1.993301	-2.302752	0.085125

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-11498.56068
Thermal Correction to Gibbs Free Energy (in a.u.)	0.098153

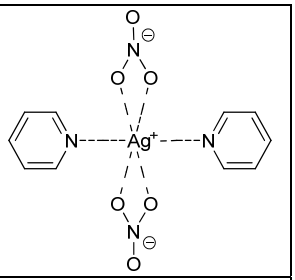
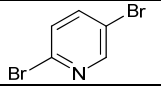
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.181571	0.022834	-0.311173
2	35	0	-5.061181	-2.466925	0.428158
3	35	0	-4.816216	2.967066	-1.299348
4	35	0	5.525624	-2.337068	-0.635851
5	35	0	5.060837	3.240740	0.478513
6	8	0	0.234779	-2.467759	0.932677
7	8	0	0.265885	-2.819112	-1.203371
8	8	0	0.345118	-4.491527	0.170505
9	8	0	-1.100749	1.962524	2.152886
10	8	0	-1.292441	-0.101649	2.778301
11	8	0	-3.060099	1.123766	2.532029
12	7	0	-1.991998	0.095945	-0.501434
13	7	0	2.351770	0.237363	-0.234223
14	7	0	0.281830	-3.262148	-0.033380
15	7	0	-1.817679	0.995161	2.492123
16	6	0	-2.713614	-0.970461	-0.135365
17	1	0	-2.163661	-1.867506	0.139824
18	6	0	-4.101933	-0.926021	-0.104288
19	6	0	-4.777656	0.238073	-0.449796
20	1	0	-5.864441	0.294469	-0.426632
21	6	0	-4.000190	1.329287	-0.818977
22	6	0	-2.613855	1.234660	-0.832500
23	1	0	-1.986628	2.077356	-1.112841
24	6	0	3.117228	-0.844665	-0.425002
25	1	0	2.605206	-1.779817	-0.640894
26	6	0	4.502873	-0.769974	-0.356718
27	6	0	5.130379	0.440362	-0.086285
28	1	0	6.214534	0.519457	-0.027900
29	6	0	4.308625	1.545053	0.105982
30	6	0	2.926707	1.418129	0.027941
31	1	0	2.265124	2.268515	0.176310

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-3042.62780
Thermal Correction to Gibbs Free Energy (in a.u.)	0.104014

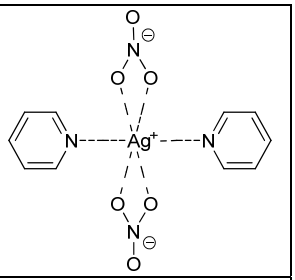
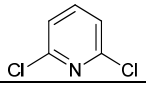
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.654389	0.951245	0.063026
2	8	0	2.218897	2.307321	1.209810
3	8	0	2.634709	2.755486	-0.867650
4	8	0	3.826830	3.661414	0.698080
5	8	0	-0.941908	-2.154564	2.069188
6	8	0	0.321894	-0.438514	2.458468
7	8	0	1.193773	-2.413887	2.300891
8	7	0	1.161091	-1.206418	-0.749438
9	7	0	-1.631923	1.344122	-0.110412
10	7	0	2.901132	2.915424	0.339088
11	7	0	0.191492	-1.672129	2.279321
12	6	0	2.347550	-1.791167	-0.652035
13	17	0	3.703608	-0.751666	-0.284990
14	6	0	2.569893	-3.152972	-0.818196
15	6	0	1.470589	-3.959403	-1.081427
16	1	0	1.589285	-5.033360	-1.210799
17	6	0	0.222196	-3.353778	-1.171008
18	6	0	0.097843	-1.982369	-1.007545
19	1	0	-0.868416	-1.488682	-1.086420
20	6	0	-2.176033	2.371752	-0.748605
21	17	0	-1.068406	3.556605	-1.399226
22	6	0	-3.542633	2.554211	-0.922958
23	6	0	-4.394754	1.592810	-0.395094
24	1	0	-5.473196	1.688155	-0.506621
25	6	0	-3.827708	0.513990	0.274792
26	6	0	-2.450610	0.413417	0.403913
27	1	0	-1.985440	-0.421545	0.927794
28	1	0	3.568674	-3.572953	-0.734776
29	17	0	-1.207102	-4.304678	-1.483715
30	1	0	-3.930534	3.418865	-1.455137
31	17	0	-4.836379	-0.732201	0.965138

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-11498.56372
Thermal Correction to Gibbs Free Energy (in a.u.)	0.099315

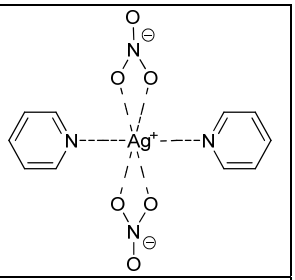
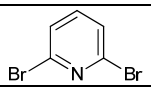
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-1.138360	-0.888750	0.220033
2	8	0	-2.799328	-1.548836	1.977433
3	8	0	-3.245080	-2.219996	-0.024448
4	8	0	-4.646232	-2.614590	1.582799
5	8	0	1.339487	1.641377	2.302382
6	8	0	-0.450831	0.478976	2.663105
7	8	0	-0.585344	2.625497	2.411006
8	7	0	-1.057516	1.332457	-0.586211
9	7	0	1.008848	-1.787094	-0.079508
10	7	0	-3.574226	-2.133766	1.181904
11	7	0	0.101533	1.584978	2.461714
12	6	0	-2.077025	2.182792	-0.582080
13	35	0	-3.801952	1.451608	-0.274332
14	6	0	-1.954879	3.550643	-0.799380
15	6	0	-0.683229	4.060036	-1.030214
16	1	0	-0.545134	5.125498	-1.204873
17	6	0	0.389020	3.174238	-1.035092
18	6	0	0.171466	1.822285	-0.808810
19	1	0	0.991154	1.106604	-0.811492
20	6	0	1.304405	-2.756309	-0.937826
21	35	0	-0.158929	-3.592464	-1.811350
22	6	0	2.597260	-3.177875	-1.226988
23	6	0	3.646881	-2.536545	-0.580757
24	1	0	4.674686	-2.833167	-0.781511
25	6	0	3.342788	-1.517631	0.316031
26	6	0	2.020044	-1.165707	0.548480
27	1	0	1.752196	-0.370003	1.244298
28	1	0	-2.821810	4.206148	-0.789840
29	35	0	2.149568	3.790168	-1.355309
30	1	0	2.788127	-3.979904	-1.935447
31	35	0	4.721926	-0.597167	1.229952

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-3042.63056
Thermal Correction to Gibbs Free Energy (in a.u.)	0.103670

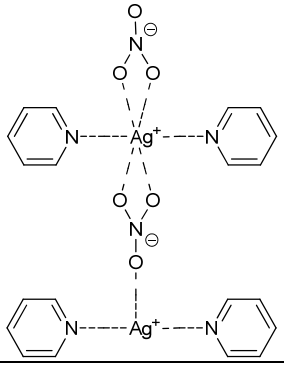
CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.719057	0.573975	0.042767
2	8	0	-1.647936	2.446307	1.371969
3	8	0	-1.232132	3.105704	-0.645214
4	8	0	-2.054533	4.495054	0.800576
5	8	0	3.026806	-1.874626	0.904465
6	8	0	4.531801	-0.761284	1.990446
7	8	0	5.107286	-2.020128	0.325036
8	7	0	1.475465	0.568126	-0.730286
9	7	0	-2.300152	-1.133964	0.215385
10	7	0	-1.647127	3.359452	0.507141
11	7	0	4.222088	-1.554907	1.075390
12	6	0	2.450386	1.222020	-0.101418
13	17	0	1.979048	2.121156	1.317190
14	6	0	3.779061	1.223298	-0.498451
15	6	0	4.108143	0.469572	-1.620546
16	1	0	5.138366	0.431280	-1.969328
17	6	0	3.117144	-0.240105	-2.291997
18	6	0	1.825559	-0.146314	-1.798326
19	17	0	0.536446	-1.007347	-2.601885
20	6	0	-3.568250	-0.979062	-0.161377
21	17	0	-3.997134	0.593415	-0.785402
22	6	0	-4.533927	-1.971454	-0.091664
23	6	0	-4.138760	-3.210328	0.403339
24	1	0	-4.859311	-4.023324	0.477631
25	6	0	-2.820187	-3.408446	0.800942
26	6	0	-1.953019	-2.333274	0.681596
27	17	0	-0.284082	-2.515125	1.154560
28	1	0	4.527043	1.783234	0.055189
29	1	0	3.337817	-0.843281	-3.168207
30	1	0	-5.554093	-1.781760	-0.414028
31	1	0	-2.476020	-4.363250	1.188578

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-11498.56524
Thermal Correction to Gibbs Free Energy (in a.u.)	0.099419

CARTESIAN COORDINATES

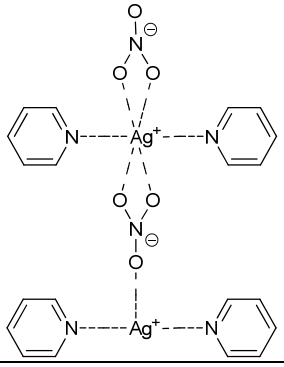
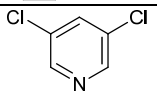
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	0.643547	0.657101	-0.262109
2	8	0	1.778140	2.254641	-1.764206
3	8	0	1.193810	3.175655	0.101468
4	8	0	2.230094	4.342538	-1.403035
5	8	0	-3.344761	-2.241140	0.250782
6	8	0	-5.232363	-1.643070	-0.623415
7	8	0	-5.122158	-2.133858	1.482221
8	7	0	-1.539072	0.726618	0.526660
9	7	0	2.164232	-1.120575	-0.337695
10	7	0	1.737432	3.269770	-1.022390
11	7	0	-4.566709	-2.009818	0.369065
12	6	0	-2.553779	1.099481	-0.252863
13	35	0	-2.122650	1.449037	-2.065906
14	6	0	-3.862626	1.243637	0.183906
15	6	0	-4.122254	0.970427	1.523417
16	1	0	-5.133399	1.068192	1.914073
17	6	0	-3.087223	0.561587	2.359261
18	6	0	-1.822351	0.456897	1.801280
19	35	0	-0.361808	-0.097226	2.877245
20	6	0	3.263731	-1.142504	0.414925
21	35	0	3.586560	0.405706	1.460908
22	6	0	4.154133	-2.205125	0.463205
23	6	0	3.870925	-3.311686	-0.331740
24	1	0	4.539034	-4.171502	-0.327612
25	6	0	2.734071	-3.316230	-1.134804
26	6	0	1.922941	-2.191847	-1.093219
27	35	0	0.359488	-2.112251	-2.163937
28	1	0	-4.653088	1.555008	-0.492913
29	1	0	-3.262754	0.331626	3.406468
30	1	0	5.036810	-2.173623	1.096258
31	1	0	2.492416	-4.165669	-1.768179

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-1847.62214
Thermal Correction to Gibbs Free Energy (in a.u.)	0.315225

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.446152	-0.638096	-1.468137
2	8	0	-1.564576	1.762648	-2.738510
3	8	0	-3.393914	2.636678	-1.980011
4	8	0	-1.480204	3.496665	-1.444919
5	8	0	1.571386	1.764339	2.736913
6	8	0	1.479415	3.496113	1.440851
7	8	0	3.396806	2.644310	1.975745
8	7	0	1.471757	0.249461	-1.803269
9	7	0	-2.309376	-1.526625	-0.914813
10	7	0	-2.146890	2.634057	-2.054309
11	7	0	2.149841	2.636981	2.051029
12	6	0	1.719831	1.455854	-1.264957
13	1	0	0.874430	1.971953	-0.813913
14	6	0	2.982198	2.033312	-1.283199
15	6	0	4.031953	1.333757	-1.872262
16	1	0	5.034905	1.757421	-1.899122
17	6	0	3.777780	0.079936	-2.421584
18	6	0	2.486895	-0.427940	-2.363437
19	1	0	2.249351	-1.404955	-2.778895
20	6	0	-3.461295	-0.864028	-1.112380
21	1	0	-3.398059	0.067431	-1.672150
22	6	0	-4.679561	-1.332492	-0.637811
23	6	0	-4.709304	-2.527432	0.075297
24	1	0	-5.648737	-2.919848	0.462145
25	6	0	-3.513785	-3.207374	0.293806
26	6	0	-2.337199	-2.672760	-0.212617
27	1	0	-1.382344	-3.172310	-0.058973
28	47	0	0.445720	-0.635152	1.469488
29	7	0	2.308130	-1.526236	0.917493
30	7	0	-1.471450	0.254631	1.803303
31	6	0	2.335226	-2.674417	0.218653
32	1	0	1.380227	-3.174466	0.067588

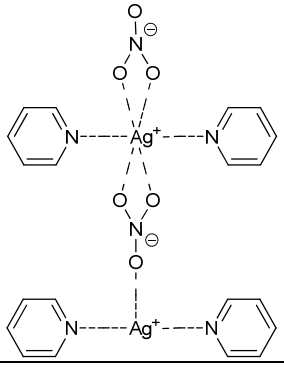
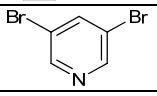
33	6	0	3.511294	-3.210464	-0.287478
34	6	0	4.707025	-2.529863	-0.072219
35	1	0	5.646052	-2.923397	-0.458919
36	6	0	4.678022	-1.332839	0.637420
37	6	0	3.460244	-0.862998	1.111854
38	1	0	3.397565	0.070196	1.668782
39	6	0	-1.719289	1.460479	1.263701
40	1	0	-0.873515	1.976550	0.813318
41	6	0	-2.981889	2.037512	1.279918
42	6	0	-4.032129	1.338117	1.868267
43	1	0	-5.035277	1.761420	1.893441
44	6	0	-3.778174	0.084910	2.419106
45	6	0	-2.487064	-0.422562	2.362961
46	1	0	-2.249702	-1.399105	2.779621
47	1	0	3.480813	-4.144876	-0.843815
48	1	0	5.583207	-0.757942	0.820915
49	1	0	4.566460	-0.508585	-2.885267
50	1	0	3.129904	3.013521	-0.836045
51	1	0	-4.567206	-0.503422	2.882425
52	1	0	-3.129399	3.017229	0.831627
53	1	0	-3.483852	-4.140148	0.852916
54	1	0	-5.584567	-0.758168	-0.823985

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5524.42946
Thermal Correction to Gibbs Free Energy (in a.u.)	0.228326

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.344442	0.118400	-1.512562
2	17	0	-4.774489	-3.231344	-0.009954
3	17	0	-5.819248	1.686004	-2.072165
4	17	0	5.295993	-0.447085	-2.379988
5	17	0	3.438214	4.292608	-0.478857
6	8	0	-0.014136	-2.318510	-2.739178
7	8	0	1.619909	-3.108983	-1.557814
8	8	0	-0.234598	-4.213283	-1.716737
9	8	0	-0.262474	-2.220147	0.921070
10	8	0	-1.433051	-3.895098	1.625679
11	8	0	-0.879498	-2.311416	2.995469
12	7	0	-2.470362	-0.314459	-1.381911
13	7	0	1.671746	0.910138	-1.542442
14	7	0	0.459398	-3.216880	-2.002986
15	7	0	-0.858322	-2.811911	1.850207
16	6	0	-2.904272	-1.471374	-0.864217
17	1	0	-2.154392	-2.207552	-0.583693
18	6	0	-4.261515	-1.715687	-0.698224
19	6	0	-5.205962	-0.765896	-1.066220
20	1	0	-6.272301	-0.941294	-0.941402
21	6	0	-4.719280	0.420321	-1.597312
22	6	0	-3.352853	0.625143	-1.741670
23	1	0	-2.960983	1.553163	-2.150862
24	6	0	2.695823	0.130293	-1.909511
25	1	0	2.464001	-0.884248	-2.227583
26	6	0	4.001230	0.605739	-1.881930
27	6	0	4.278153	1.899766	-1.460817
28	1	0	5.294423	2.287267	-1.436730
29	6	0	3.192872	2.670176	-1.063841
30	6	0	1.903402	2.157194	-1.111235
31	1	0	1.045802	2.752856	-0.807330
32	47	0	0.400914	0.287678	1.610627

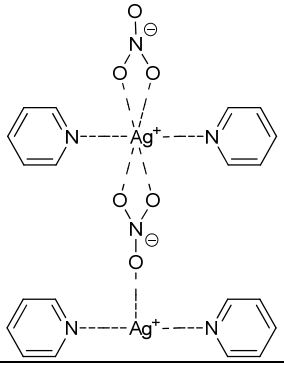
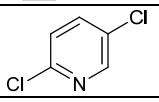
33	17	0	-3.246564	4.395170	-0.013686
34	17	0	-5.275398	0.002782	2.459527
35	17	0	4.692997	-3.345678	0.489840
36	17	0	5.951666	1.761097	1.853836
37	7	0	-1.593955	1.162047	1.570917
38	7	0	2.525522	-0.204177	1.554118
39	6	0	-1.783495	2.338798	0.960205
40	1	0	-0.902292	2.866775	0.604360
41	6	0	-3.058215	2.864996	0.797397
42	6	0	-4.173101	2.178174	1.260284
43	1	0	-5.178889	2.577790	1.148323
44	6	0	-3.940250	0.950545	1.866443
45	6	0	-2.647260	0.461015	2.006676
46	1	0	-2.448647	-0.496200	2.484678
47	6	0	2.907387	-1.429207	1.169992
48	1	0	2.124607	-2.168212	1.014018
49	6	0	4.249640	-1.737162	0.989577
50	6	0	5.233108	-0.778881	1.197693
51	1	0	6.288569	-1.003397	1.059192
52	6	0	4.799623	0.480847	1.587551
53	6	0	3.446320	0.745696	1.756205
54	1	0	3.096434	1.730188	2.057016

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-22436.30830
Thermal Correction to Gibbs Free Energy (in a.u.)	0.216333

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.190003	0.128132	-1.542455
2	35	0	-4.591681	-3.613483	-0.590635
3	35	0	-5.796950	1.778735	-2.011901
4	35	0	5.562006	-0.760377	-2.231958
5	35	0	3.708890	4.397670	-0.643726
6	8	0	0.208239	-2.268520	-2.852197
7	8	0	1.711583	-3.156634	-1.569861
8	8	0	-0.144034	-4.203773	-1.947982
9	8	0	-0.384176	-2.458007	0.794403
10	8	0	-0.875553	-4.408457	1.586088
11	8	0	-1.046914	-2.655402	2.846747
12	7	0	-2.311791	-0.330787	-1.517617
13	7	0	1.855017	0.835021	-1.496459
14	7	0	0.594491	-3.213316	-2.122194
15	7	0	-0.769952	-3.176805	1.745447
16	6	0	-2.723322	-1.559492	-1.179801
17	1	0	-1.955706	-2.303954	-0.983810
18	6	0	-4.075736	-1.863043	-1.081094
19	6	0	-5.036952	-0.891786	-1.334596
20	1	0	-6.100251	-1.113597	-1.271247
21	6	0	-4.576550	0.375257	-1.672943
22	6	0	-3.212980	0.629937	-1.755056
23	1	0	-2.830367	1.611921	-2.022390
24	6	0	2.864042	0.006839	-1.793486
25	1	0	2.602919	-1.022203	-2.037264
26	6	0	4.181055	0.451987	-1.787147
27	6	0	4.479784	1.770554	-1.463599
28	1	0	5.503225	2.140677	-1.468867
29	6	0	3.410917	2.595617	-1.131579
30	6	0	2.111347	2.103718	-1.152167
31	1	0	1.258732	2.729848	-0.900237
32	47	0	0.167563	0.003833	1.527569

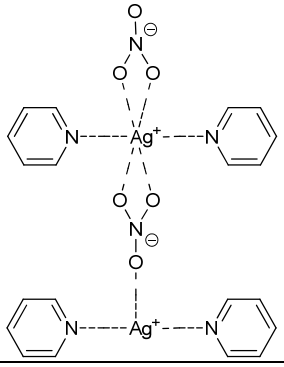
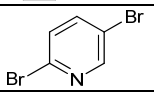
33	35	0	-3.602705	4.416220	0.545375
34	35	0	-5.611358	-0.618654	2.315151
35	35	0	4.755285	-3.601532	0.809888
36	35	0	5.719923	1.876733	2.040465
37	7	0	-1.851033	0.841214	1.554071
38	7	0	2.322419	-0.381581	1.573119
39	6	0	-2.069429	2.102225	1.161328
40	1	0	-1.197519	2.694920	0.894706
41	6	0	-3.355320	2.627852	1.107292
42	6	0	-4.449618	1.845162	1.457227
43	1	0	-5.463110	2.240729	1.433729
44	6	0	-4.190509	0.533109	1.836630
45	6	0	-2.885907	0.054359	1.872136
46	1	0	-2.653938	-0.966827	2.171144
47	6	0	2.786509	-1.602189	1.275629
48	1	0	2.047023	-2.379215	1.095268
49	6	0	4.151612	-1.856978	1.210017
50	6	0	5.069370	-0.838979	1.441069
51	1	0	6.141505	-1.020136	1.398464
52	6	0	4.555730	0.419091	1.731649
53	6	0	3.182169	0.621023	1.792883
54	1	0	2.758318	1.594135	2.028608

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5524.44158
Thermal Correction to Gibbs Free Energy (in a.u.)	0.224512

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.324410	-0.185667	-1.590494
2	8	0	-0.992755	2.469899	-1.110040
3	8	0	-0.976344	1.960804	-3.213052
4	8	0	-1.298014	4.012785	-2.597783
5	8	0	0.965863	2.125781	1.481262
6	8	0	2.383516	2.861027	2.940439
7	8	0	0.349768	2.416738	3.538192
8	7	0	1.833601	0.241987	-1.759791
9	7	0	-2.411888	-0.895654	-1.409726
10	7	0	-1.089035	2.819232	-2.308806
11	7	0	1.231699	2.471223	2.656666
12	6	0	2.235570	1.484129	-1.447171
13	1	0	1.466982	2.184929	-1.130745
14	6	0	3.568957	1.853734	-1.532281
15	6	0	4.525219	0.936306	-1.953532
16	1	0	5.574523	1.210949	-2.037679
17	6	0	4.106108	-0.351581	-2.260943
18	6	0	2.752651	-0.640434	-2.142313
19	17	0	2.186580	-2.243499	-2.525010
20	6	0	-3.384821	0.028908	-1.370068
21	1	0	-3.084353	1.067098	-1.487927
22	6	0	-4.710951	-0.326255	-1.184223
23	6	0	-5.062505	-1.660883	-1.012810
24	1	0	-6.097409	-1.956997	-0.853921
25	6	0	-4.053178	-2.612900	-1.052643
26	6	0	-2.751189	-2.173025	-1.258928
27	17	0	-1.459585	-3.336910	-1.339746
28	47	0	0.267638	-0.547508	1.454933
29	7	0	2.360351	-1.172841	1.278239
30	7	0	-1.836962	-0.031064	1.770751
31	6	0	2.730649	-2.423988	1.014193
32	17	0	1.464984	-3.617849	0.966655

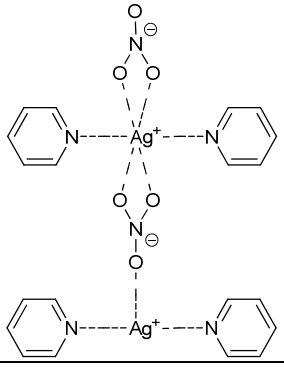
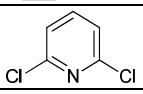
33	6	0	4.045200	-2.813858	0.790976
34	6	0	5.034341	-1.842973	0.867920
35	1	0	6.078086	-2.102762	0.703518
36	6	0	4.650962	-0.539499	1.164097
37	6	0	3.314173	-0.228711	1.350634
38	1	0	2.989267	0.787973	1.559309
39	6	0	-2.188168	1.252281	1.589652
40	1	0	-1.389679	1.945090	1.337718
41	6	0	-3.502702	1.666331	1.733227
42	6	0	-4.492760	0.753617	2.078663
43	1	0	-5.527782	1.063007	2.207706
44	6	0	-4.125897	-0.575085	2.250328
45	6	0	-2.788435	-0.908715	2.080914
46	17	0	-2.286904	-2.563180	2.297209
47	1	0	4.289586	-3.848657	0.567724
48	17	0	5.837733	0.729425	1.291449
49	17	0	4.024013	3.479323	-1.101367
50	1	0	4.812157	-1.109959	-2.587052
51	1	0	-4.860317	-1.331342	2.511840
52	17	0	-3.888856	3.344389	1.468237
53	1	0	-4.272819	-3.669679	-0.927749
54	17	0	-5.925022	0.922934	-1.153251

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-22436.31543
Thermal Correction to Gibbs Free Energy (in a.u.)	0.216058

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.345872	-0.148205	1.571519
2	8	0	-0.050560	1.970845	3.281564
3	8	0	1.078814	3.480491	2.215361
4	8	0	-0.952959	3.887999	2.839295
5	8	0	0.127352	1.755077	-0.381560
6	8	0	-0.917203	3.640383	-0.557609
7	8	0	-0.383780	2.526901	-2.337848
8	7	0	-2.523826	0.188875	1.445160
9	7	0	1.825689	-0.544138	1.727617
10	7	0	0.025977	3.117355	2.777269
11	7	0	-0.393095	2.648653	-1.094095
12	6	0	-2.914232	1.434337	1.118933
13	1	0	-2.129317	2.170877	0.961858
14	6	0	-4.255974	1.765990	0.998980
15	6	0	-5.231956	0.792097	1.186436
16	1	0	-6.291650	1.019965	1.090294
17	6	0	-4.824633	-0.495033	1.511713
18	6	0	-3.461697	-0.735526	1.640617
19	35	0	-2.873034	-2.460192	2.154651
20	6	0	2.626372	0.534228	1.644107
21	1	0	2.136532	1.502404	1.550356
22	6	0	4.007288	0.417096	1.709447
23	6	0	4.595621	-0.838709	1.824708
24	1	0	5.676006	-0.962671	1.861286
25	6	0	3.765203	-1.948585	1.909360
26	6	0	2.391382	-1.741695	1.870422
27	35	0	1.232108	-3.224171	2.068103
28	47	0	0.380920	-0.625057	-1.590898
29	7	0	-1.761802	-1.123639	-1.739709
30	7	0	2.552739	-0.247563	-1.743472
31	6	0	-2.288764	-2.327065	-1.517088
32	35	0	-1.082146	-3.747396	-1.197239

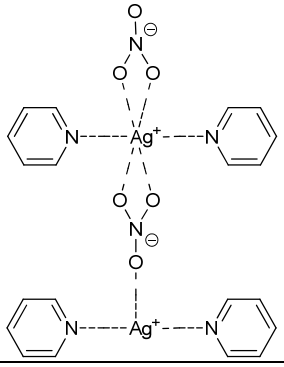
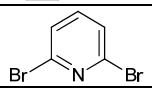
33	6	0	-3.654264	-2.586297	-1.529300
34	6	0	-4.517012	-1.537296	-1.818571
35	1	0	-5.591430	-1.707367	-1.845155
36	6	0	-3.968102	-0.285902	-2.082054
37	6	0	-2.594778	-0.104760	-2.016570
38	1	0	-2.131958	0.861405	-2.206673
39	6	0	2.909791	1.044873	-1.838183
40	1	0	2.098802	1.766697	-1.895603
41	6	0	4.240215	1.432719	-1.878289
42	6	0	5.245410	0.475441	-1.781727
43	1	0	6.299132	0.747768	-1.797408
44	6	0	4.873465	-0.858800	-1.673409
45	6	0	3.516804	-1.163705	-1.673837
46	35	0	2.977996	-2.977609	-1.608120
47	1	0	-5.553855	-1.284786	1.669852
48	35	0	-4.738719	3.546628	0.589952
49	1	0	4.182330	-2.946305	2.014408
50	35	0	5.072999	1.978260	1.672100
51	1	0	5.626371	-1.638897	-1.600481
52	35	0	4.655648	3.265790	-2.074995
53	1	0	-4.040480	-3.581991	-1.329166
54	35	0	-5.072900	1.172556	-2.555310

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-5524.43096
Thermal Correction to Gibbs Free Energy (in a.u.)	0.222113

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-0.819607	2.308783	-0.145444
2	8	0	-1.145490	4.655527	-1.227788
3	8	0	0.650790	3.601952	-1.808391
4	8	0	0.242537	5.569572	-2.618389
5	8	0	-0.607930	2.694065	2.102518
6	8	0	0.944566	4.095560	1.524120
7	8	0	0.566373	3.687657	3.616937
8	7	0	3.806127	0.033159	-1.165200
9	7	0	-1.786451	0.724236	-1.516426
10	7	0	-0.081860	4.615990	-1.890231
11	7	0	0.313626	3.505098	2.414541
12	6	0	4.266700	0.796626	-0.187321
13	17	0	3.130136	1.950215	0.481024
14	6	0	5.557557	0.741019	0.324621
15	6	0	6.417416	-0.198433	-0.236862
16	1	0	7.440033	-0.288697	0.125843
17	6	0	5.963733	-1.028605	-1.258593
18	6	0	4.647612	-0.855341	-1.666748
19	17	0	4.010159	-1.874415	-2.946022
20	6	0	-3.104889	0.669888	-1.695720
21	17	0	-4.019497	2.005574	-1.042692
22	6	0	-3.763410	-0.350414	-2.364175
23	6	0	-2.982087	-1.382734	-2.875026
24	1	0	-3.452344	-2.212113	-3.400113
25	6	0	-1.600595	-1.352088	-2.712986
26	6	0	-1.063058	-0.270214	-2.031140
27	17	0	0.661718	-0.148407	-1.816495
28	47	0	-0.734008	-1.843649	1.015419
29	7	0	1.455316	-1.939910	1.243052
30	7	0	-2.924387	-1.891984	0.793064
31	6	0	2.193939	-2.793422	0.527198
32	17	0	1.338449	-3.751201	-0.646283

33	6	0	3.560778	-2.957124	0.681418
34	6	0	4.195068	-2.174102	1.640056
35	1	0	5.267637	-2.267876	1.797743
36	6	0	3.457807	-1.262921	2.389192
37	6	0	2.096280	-1.190041	2.145423
38	17	0	1.112559	-0.076024	3.047572
39	6	0	-3.686838	-0.901905	1.269195
40	17	0	-2.865203	0.313690	2.202203
41	6	0	-5.054709	-0.807607	1.069661
42	6	0	-5.664675	-1.813857	0.328254
43	1	0	-6.736471	-1.781310	0.142013
44	6	0	-4.901757	-2.863541	-0.172443
45	6	0	-3.541944	-2.846997	0.091234
46	17	0	-2.537622	-4.138289	-0.501783
47	1	0	4.106461	-3.672277	0.072584
48	1	0	3.922767	-0.627348	3.137217
49	1	0	5.873630	1.399094	1.129391
50	1	0	6.603482	-1.778270	-1.716222
51	1	0	-5.345080	-3.668216	-0.751920
52	1	0	-5.619577	0.023840	1.481231
53	1	0	-0.959856	-2.137649	-3.103310
54	1	0	-4.843587	-0.339822	-2.476224

Complex:	
Ligand:	
Total electronic energy (in a.u.)	-22436.30017
Thermal Correction to Gibbs Free Energy (in a.u.)	0.212606

CARTESIAN COORDINATES

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	47	0	-1.783428	-1.242941	-0.004411
2	8	0	-3.527944	-3.084642	-1.045762
3	8	0	-3.149058	-1.179369	-1.993691
4	8	0	-4.282967	-2.697982	-3.039992
5	8	0	-1.422459	-1.481590	2.250910
6	8	0	-2.888964	-3.077360	2.156152
7	8	0	-2.010928	-2.511805	4.053430
8	7	0	-4.953675	1.452010	-0.371233
9	7	0	0.110017	-0.855516	-1.459273
10	7	0	-3.661337	-2.330802	-2.030117
11	7	0	-2.117947	-2.370368	2.824041
12	6	0	-5.281647	0.289218	0.171467
13	35	0	-6.589591	-0.736522	-0.757523
14	6	0	-4.769306	-0.202276	1.367267
15	6	0	-3.862033	0.606849	2.046302
16	1	0	-3.442329	0.280545	2.995880
17	6	0	-3.501114	1.838252	1.506496
18	6	0	-4.078022	2.188191	0.293110
19	35	0	-3.609812	3.862974	-0.495098
20	6	0	0.944513	-1.845990	-1.764500
21	35	0	0.343762	-3.597172	-1.341680
22	6	0	2.163327	-1.672623	-2.406857
23	6	0	2.506738	-0.375846	-2.778957
24	1	0	3.441699	-0.186940	-3.303613
25	6	0	1.633475	0.674986	-2.511946
26	6	0	0.452957	0.370350	-1.846480
27	35	0	-0.814951	1.741075	-1.502748
28	47	0	2.925911	0.566881	0.775939
29	7	0	1.879116	2.533225	0.816367
30	7	0	3.819733	-1.449016	0.504279
31	6	0	2.288582	3.571903	0.076439
32	35	0	3.896555	3.340033	-0.893915

33	6	0	1.619322	4.782458	-0.006814
34	6	0	0.458500	4.929738	0.745702
35	1	0	-0.096001	5.865899	0.717370
36	6	0	0.010780	3.874227	1.530870
37	6	0	0.747796	2.699195	1.516346
38	35	0	0.128509	1.200617	2.478176
39	6	0	3.167846	-2.543802	0.921305
40	35	0	1.641759	-2.258073	1.993756
41	6	0	3.541774	-3.838602	0.593693
42	6	0	4.656558	-4.005042	-0.219714
43	1	0	4.980541	-5.003725	-0.506954
44	6	0	5.360397	-2.888614	-0.659085
45	6	0	4.899748	-1.643559	-0.262599
46	35	0	5.840274	-0.096190	-0.811711
47	1	0	-2.813258	2.504121	2.018894
48	1	0	-5.072192	-1.168337	1.761658
49	1	0	1.854903	1.690274	-2.828773
50	1	0	2.814683	-2.515529	-2.623041
51	1	0	6.240515	-2.987017	-1.288168
52	1	0	2.978216	-4.691846	0.960321
53	1	0	1.993984	5.588606	-0.631476
54	1	0	-0.889087	3.963995	2.133046
