Published in "Chemistry - A European Journal 19(5): 1754–1761, 2013"
which should be cited to refer to this work.

Table S1. Crystal data and structure refinement details for **1-3**.

	1	**2**	**3**
Formula	$C_{24}H_{38}Ag_2N_{14}O_{15}$	$C_{12}H_{22}Ag_2N_{10}O_{17}$	$C_6H_{10}AgN_5O_8$
*M*r	978.42	794.14	388.06
T [K]	150(2)	150(2)	150(2)
wavelength [Å]	0.71073	0.71073	0.71073
crystal system	orthorhombic	triclinic	triclinic
space group	$P2_12_12$ (Nr. 18)	$P\bar{1}$ (Nr. 1)	$P\bar{1}$ (Nr. 2)
a [Å]	33.66280(10)	5.09440(10)	5.1720(2)
b [Å]	9.7125(3)	9.1670(3)	8.3581(3)
c [Å]	5.2157(8)	13.1855(4)	13.5530(5)
α [°]	90	77.470(2)	94.146(3)
β [°]	90	82.912(2)	95.462(3)
γ [°]	90	79.988(2)	93.181(3)
V [Å^3]	1705.3(3)	589.59(3)	580.54(4)
Z	4	1	2
ρ_{calcd} [Mgm^{-3}]	1.906	2.237	2.220
μ(Mo-Kα) [mm^{-1}]	1.241	1.727	1.789
F(000)	988	394	384
θ range [°]	2.18-19.98	2.30-27.50	2.98-23.99
index ranges	$-32 \le h \le 32$	$-6 \le h \le 6$	$-5 \le h \le 5$
	$-9 \le k \le 9$	$-11 \le k \le 11$	$-9 \le k \le 9$
	$-4 \le l \le 5$	$-17 \le l \le 17$	$-15 \le l \le 15$
reflections collected	6610	17644	10061
unique reflections	1563	5172	1809
	R(int) = 0.0412	*R(int)* = 0.1654	*R(int)* = 0.0454
completeness to θ	98.6%	99.9%	99.5%
refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
data / restraints / parameters	1563 / 0 / 255	5172 / 3 / 374	1809 / 0 / 182
Goodness-of-fit on F^2	1.072	1.064	1.128
Final R indices [I>2sigma(I)]	*R1* = 0.0153	*R1* = 0.0477	*R1* = 0.0153
	wR2 = 0.0346	*wR2* = 0.1133	*wR2* = 0.0342
R indices (all data)	*R1* = 0.0161	*R1* = 0.0486	*R1* = 0.0163
	wR2 = 0.0347	*wR2* = 0.1145	*wR2* = 0.0345
Largest diff. peak and hole	0.150 and –0.259 e.Å^{-3}	1.699 and –1.362 e.Å^{-3}	0.258 and –0.360 e.Å^{-3}
Flack-parameter	-0.03(2)	-0.05(3)	

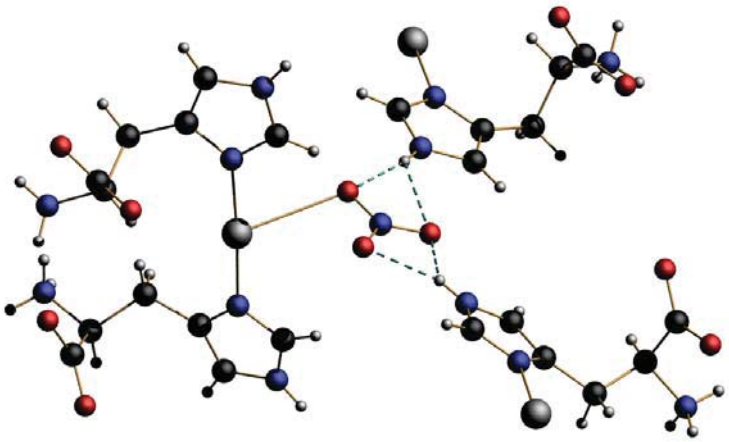

Figure S1. View of the intermolecular hydrogen bonding network in **1** indicated by the dashed blue lines. Color code: black: carbon, red: oxygen, blue: nitrogen, silver: silver.

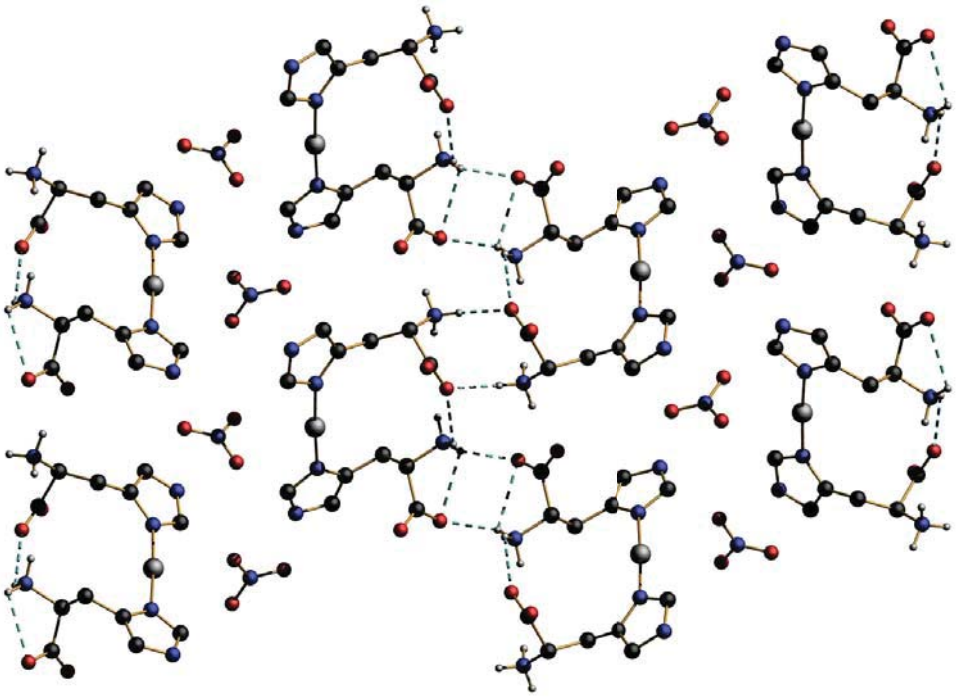

Figure S2. Packing in **1** resulting from hydrogen bonding indicated by the dashed blue lines; view along the *c*-axis. Most hydrogen atoms and the water molecules have been omitted for clarity. Color code: black: carbon, red: oxygen, blue: nitrogen, silver: silver.

Table S2. Detailed description of the hydrogen bonding network in **1**. Bond lengths are given in Å and torsion angles in °.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1)#1	0.89	2.05	2.817(3)	144.4
N(1)-H(1B)...O(1W)#2	0.89	2.20	2.915(4)	136.5
N(1)-H(1B)...O(4)	0.89	2.50	3.046(4)	119.9
N(1)-H(1C)...O(3)#3	0.89	1.85	2.737(3)	172.1
N(3)-H(3)...O(2N)#4	0.86	2.01	2.847(4)	164.7
N(3)-H(3)...O(3N)#4	0.86	2.38	3.040(4)	134.0
N(4)-H(4A)...O(4)#5	0.89	1.95	2.836(4)	175.9
N(4)-H(4B)...O(2)#6	0.89	1.81	2.689(3)	169.1
N(4)-H(4C)...O(3)#3	0.89	1.95	2.841(4)	173.8
N(6)-H(6A)...O(1N)#7	0.86	2.05	2.888(4)	163.5
N(6)-H(6A)...O(3N)#7	0.86	2.39	2.986(4)	127.0
O(1W)-H(1W)...O(1)#8	0.81(4)	2.00(4)	2.782(4)	162(4)

Symmetry transformations used to generate equivalent atoms: #1: -x+1,-y+2, z; #2: x,y+1, z; #3: x,y,z+1; #4: -x+1/2, y+1/2, -z+2; #5: -x+1, -y+1, z; #6: x, y-1, z; #7: -x+1/2, y-1/2, -z; #8: x, y-1, z-1.

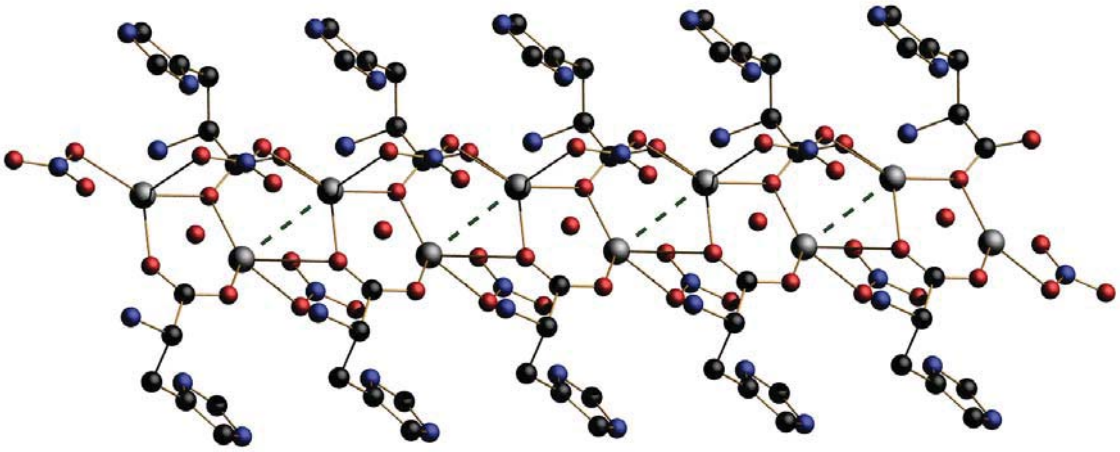

Figure S3. 1-D chain in **2** evolving horizontally along *a*-axis. Hydrogen atoms and intercalating nitrate molecules have been omitted for clarity. The Ag-Ag interactions are indicated by dashed green lines. Color code: black: carbon, red: oxygen, blue: nitrogen, silver: silver.

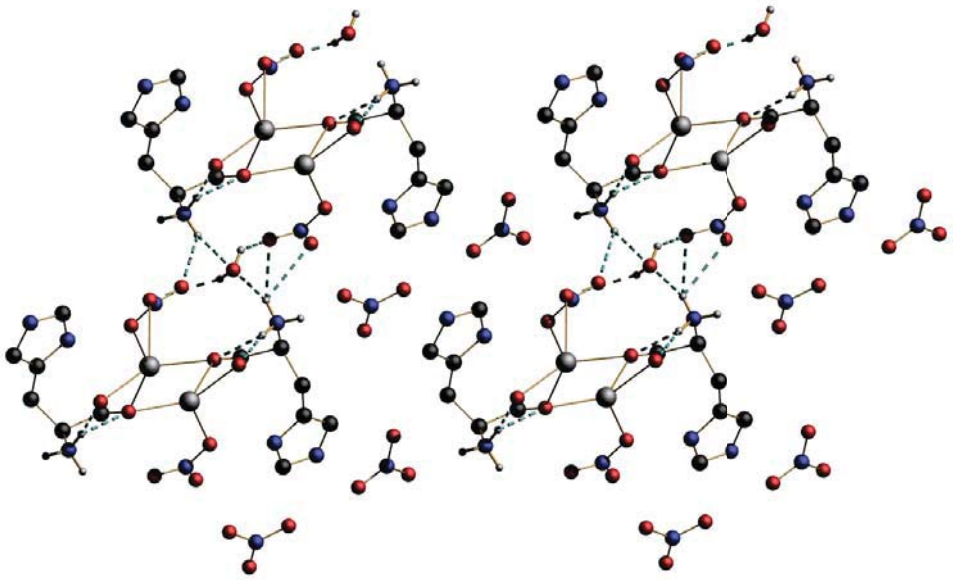

Figure S4. Organization of the packing in between chains in **2** with nitrate and water molecules (view down the crystallographic *a*-axis). The hydrogen bonding network is indicated by the dashed blue lines. Most Hydrogen atoms are omitted for more clarity. Color code: black: carbon, red: oxygen, blue: nitrogen, silver: silver.

Table S3. Detailed description of the hydrogen bonding network in **2**. Bond lengths are given in Å and torsion angles in °.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1W)	0.89	2.09	2.878(6)	146.3
N(1)-H(1A)...O(2N)#3	0.89	2.50	3.096(8)	124.5
N(1)-H(1A)...O(3N)#3	0.89	2.50	3.001(9)	116.1
N(1)-H(1B)...O(10N)#4	0.89	2.44	3.263(11)	153.6
N(1)-H(1B)...O(12N)#4	0.89	2.25	3.071(14)	153.1
N(1)-H(1C)...O(1)#2	0.89	1.99	2.871(6)	169.2
N(2)-H(2A)...O(1N)#2	0.86	1.92	2.782(9)	175.8
N(2)-H(2A)...O(3N)#2	0.86	2.41	2.991(8)	125.3
N(3)-H(3)...O(8N)#1	0.86	1.93	2.791(7)	174.4
N(4)-H(4A)...O(1W)#5	0.89	2.01	2.828(6)	153.0
N(4)-H(4A)...O(5N)#5	0.89	2.51	2.963(7)	112.5
N(4)-H(4B)...O(9N)#6	0.89	2.02	2.837(8)	152.9
N(4)-H(4C)...O(4)#2	0.89	1.99	2.866(6)	166.7
N(5)-H(5A)...O(4N)#1	0.86	1.98	2.819(8)	163.5
N(6)-H(6A)...O(8N)#7	0.86	2.53	3.079(7)	122.6

N(6)-H(6A)...O(11N)#7	0.86	1.97	2.801(7)	162.6
O(1W)-H(1WA)...O(5N)#1	0.814(5)	2.226(7)	3.017(9)	164.2(4)
O(1W)-H(1WA)...O(6N)#	0.814(5)	2.511(7)	3.103(8)	130.7(3)
O(1W)-H(1WB)...O(2N)#4	0.768(5)	2.277(6)	2.808(7)	127.0(4)
O(1W)-H(1WB)...O(3)#4	0.768(5)	2.605(5)	3.260(7)	144.3(3)

Symmetry transformations used to generate equivalent atoms: #1: x-1, y, z; #2: x+1, y, z; #3: x+1, y+1, z; #4: x, y+1, z; #5: x, y-1, z ; #6 : x, y-1, z+1; #7: x, y, z+1.

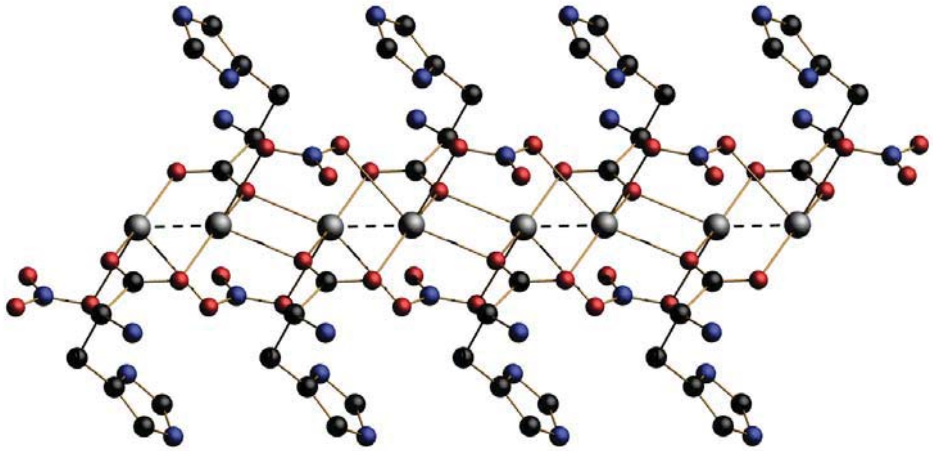

Figure S5. 1-D chain in **3** evolving horizontally along the *a*-axis. Hydrogen atoms and intercalating nitrate molecules have been omitted for clarity. The Ag-Ag interactions are indicated by dashed green lines. Color code: black: carbon, red: oxygen, blue: nitrogen, silver: silver.

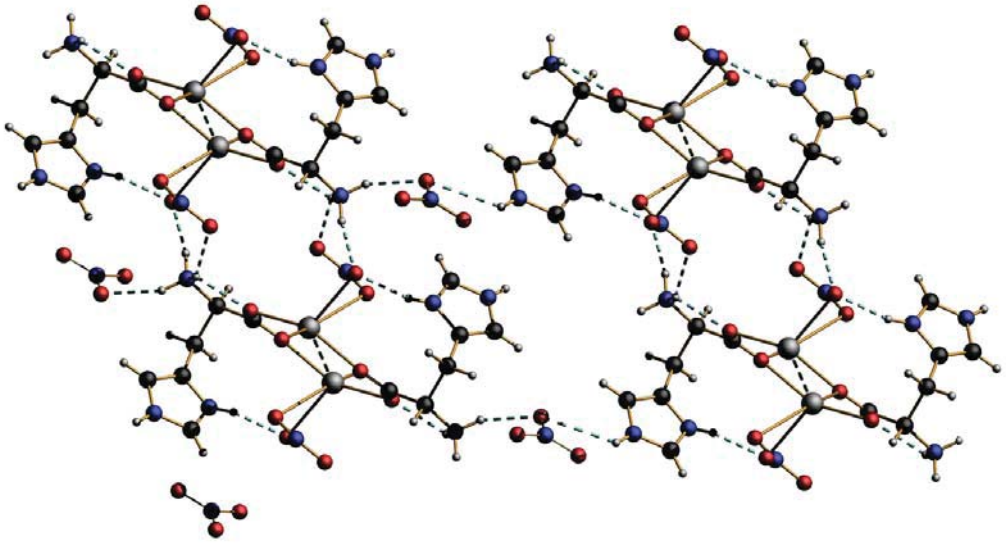

Figure S6. Organization of the packing in between chains with nitrate molecules for **3** (viewing along *a*-axis). Most hydrogen atoms have been omitted for clarity. The Ag-Ag interactions are indicated by dashed green lines while the hydrogen bonding network is indicated by dashed blue lines. Color code: black: carbon, red: oxygen, blue: nitrogen, silver: silver.

Table S4. Detailed description of the hydrogen bonding network in **3**. Bond lengths are given in Å and torsion angles in °.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(2)	0.89	2.11	2.634(2)	116.5
N(1)-H(1A)...O(2N)#3	0.89	2.21	2.937(2)	138.4
N(1)-H(1B)...O(1N)#4	0.89	1.93	2.807(2)	169.1
N(1)-H(1C)...O(4N)#4	0.89	2.13	2.922(2)	148.3
N(2)-H(2A)...O(1N)	0.86	1.95	2.792(2)	164.9
N(3)-H(3)...O(6N)#5	0.86	1.94	2.792(2)	172.0

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

Table S5. Composition of the complex structures used for calculations.

Complex	# Ag^+	# His[a]	# NO_3^-	Charge	Spin
[Ag(L-Histidine)$_2$$NO_3$]$_2$$H_2O$ **1**	3	6	3	0	Singlet
{[Ag(L-Histidinium)(NO_3)$_2$]$_2$$H_2O$}$_n$ **2**	6	6	6	6	Singlet
{Ag_2(L-Histidinium)(D-Histidinium)(NO_3)$_4$}$_n$ **3**	6	6	6	6	Singlet

[a] In the complex structures, histidine is in singly protonated state (at the π-position) for complex **1** and a doubly protonated state for complex **2** and **3**. In addition, a neutral structure was produced with a singly protonated histidine at the π-position for **1** and at the τ-position for structures **2** and **3**.