Interaction of tripodal Schiff-base ligands with silver(I): Structural and solution studies

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Crystallography

[Ag(1)]ClO_4

Table S1. Selected angles [°] of [Ag(**1**)]ClO_4

atom	angle [°]	atom	angle [°]
N1-Ag1-N2	76.65	N2-Ag1-N3	114.89
N1-Ag1-N3	76.65	N2-Ag1-N4	117.13
N1-Ag1-N4	76.72	N3-Ag1-N4	112.53

Table S2. CH···O and CH···π interactions in [Ag(**1**)]ClO_4

C-H	A	C-H [Å]	H···A [Å]	C···A [Å]	C-H···A [°]
C25-H25A	O1^{i}	0.95	2.55	3.1927	125
C11-H11B	Cg2^{ii}	0.99	2.83	3.8004	168
C23-H23A	Cg1^{iii}	0.95	2.93	3.7998	154

Symmetry codes: (i) = 1-x,1-y,1-z, (ii) = 2-x,-y,1-z, (iii) = 2-x,1-y,1-z,

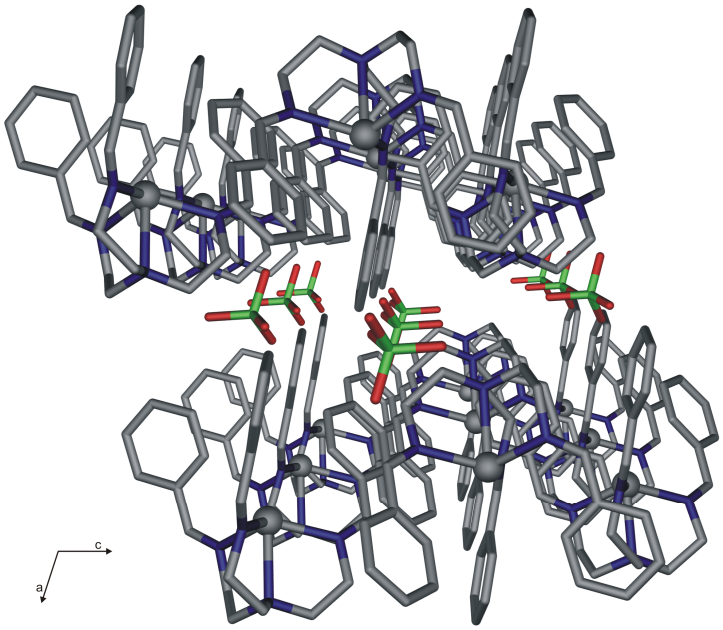

Fig. S1 Crystal packing in [Ag(**1**)]ClO_4, viewed along *b*-axis.

[Ag(2)]ClO_4

Table S3. Selected angles [°] of [Ag(**2**)]ClO4

atom	angle [°]	atom	angle [°]
N1-Ag1-N4	76.74	N4-Ag1-N20	115.63
N1-Ag1-N20	75.88	N4-Ag1-N36	119.09
N1-Ag1-N36	77.41	N20-Ag1-N36	109.81

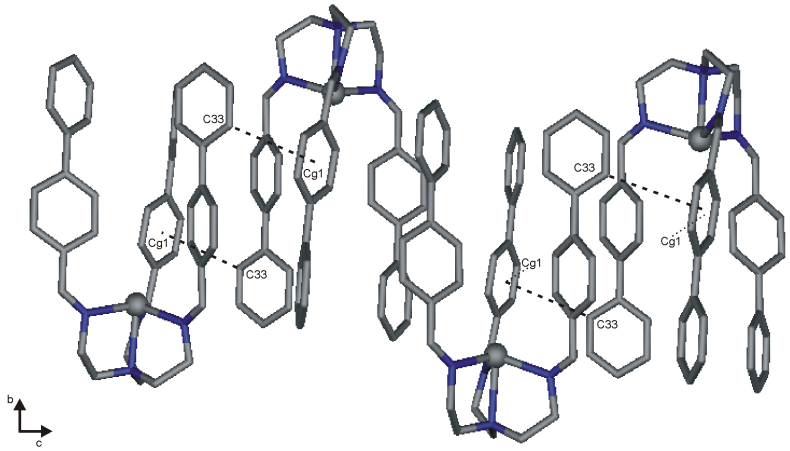

Fig. S2. CH···π-interaction in [Ag(**2**)]ClO_4, H atoms and ClO_4^- counter ion removed for clarity, projection along the a-axis.

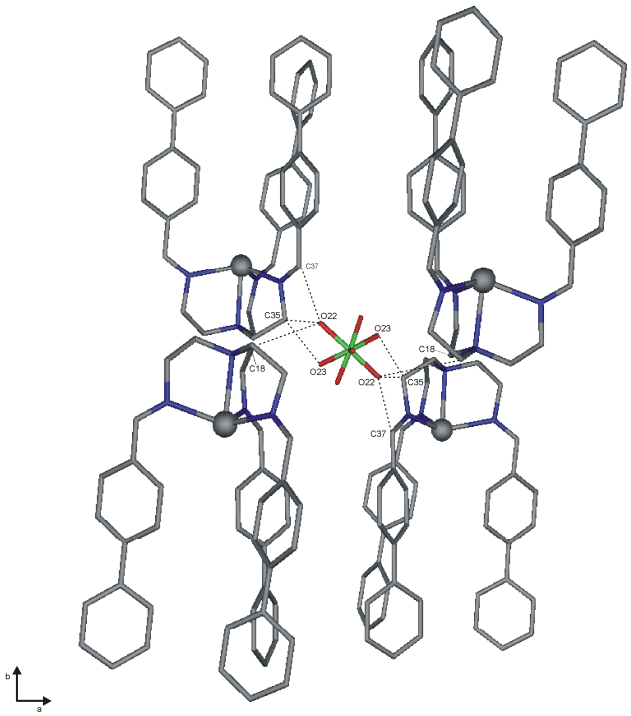

Fig. S3. CH···O-interaction in [Ag(**2**)]ClO_4, H atoms removed for clarity, viewed along *c*-axis.

Table S4. H-bond interactions in[Ag(**2**)] ClO_4

D-H···A	D-H [Å]	H···A [Å]	D···A [Å]	D-H-A [°]
C18-H18A ···· O22'[i]	0.99	2.51	3.133(7)	120
C35-H35B ···· O22[ii]	0.99	2.42	3.339(7)	154
C35-H35B ···· O23[iii]	0.99	2.50	3.472(9)	169
C37-H37 ···· O22[ii]	0.95	2.31	3.148(7)	146

symmetry: i = 3/2-x,1/2-y,z; ii = 3/2-x,y,1/2+z; iii = x,1/2-y,1/2+z

$[Ag_3(3)_2](ClO_4)_3 \cdot 0.5H_2O$

Table S5. Selected bond lengths [Å] and angles [°] of $[Ag_3(\mathbf{3})_2](ClO_4)_3 \cdot 0.5H_2O$

atom	bond length [Å]	atom	angle [°]	atom	angle [°]
Ag(1)-N(2)	2.270(6)	N(2)-Ag(1)-N(3)	70.97	N(3)-Ag(1)-N(5)	103.89
Ag(1)-N(3)	2.481(6)	N(2)-Ag(1)-N(4)	117.04	N(4)-Ag(1)-N(5)	71.49
Ag(1)-N(4)	2.307(7)	N(2)-Ag(1)-N(5)	171.41		
Ag(1)-N(5)	2.375(7)	N(3)-Ag(1)-N(4)	136.20		
Ag(2)-N(6)	2.355(6)	N(6)-Ag(2)-N(7)	71.68	N(7)-Ag(2)-N(10)	97.32
Ag(2)-N(7)	2.366(6)	N(6)-Ag(2)-N(9)	126.14	N(9)-Ag(2)-N(10)	71.41
Ag(2)-N(9)	2.276(6)	N(6)-Ag(2)-N(10)	153.66		
Ag(2)-N(10)	2.469(6)	N(7)-Ag(2)-N(9)	158.15		
Ag(3)-N(11)	2.324(6)	N(11)-Ag(3)-N(12)	72.18	N(12)-Ag(3)-N(14)	103.77
Ag(3)-N(12)	2.345(6)	N(11)-Ag(3)-N(13)	119.37	N(13)-Ag(3)-N(14)	71.57
Ag(3)-N(13)	2.286(6)	N(11)-Ag(3)-N(14)	142.42		
Ag(3)-N(14)	2.457(7)	N(12)-Ag(3)-N(13)	166.61		

The crystal packing of $[Ag_3(\mathbf{3})_2](ClO_4)_3 \cdot 0.5H_2O$ is shown in Fig. S4 together with the H-bond pattern. The H-atoms of the coordinated water molecule was not observed. However, a separation of 3.02 Å between the water O-atom (OW1) and O-atom O1 of one ClO_4^- ion is indicative of the presence of a H-bond.

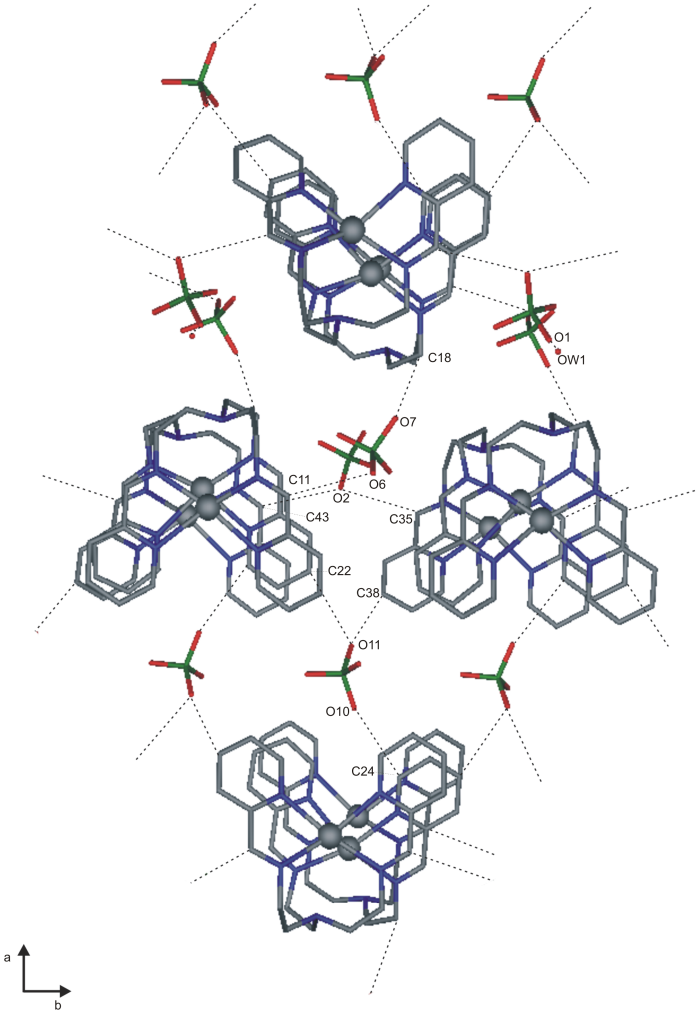

Fig. S4. H-bonding in $[Ag_3(\mathbf{3})_2](ClO_4)_3 \cdot 0.5H_2O$ viewed along the *c*-axis. H atoms and the disorder of the ClO_4^- anion are omitted for clarity.

Table S6. Selected bond lengths and angles of CH···O and O-water interaction in $[Ag_3(\mathbf{3})_2](ClO_4)_3 \cdot 0.5H_2O$.

D-H···A	D-H [Å]	H···A [Å]	D···A [Å]	D-H-A [°]
C11 – H11A ···· O6 [i]	0.95	2.41	3.259(15)	148
C18 – H18A ···· O7 [ii]	0.99	2.41	3.264(13)	144
C22 – H22A ···· O11 [iii]	0.95	2.46	3.268(19)	142
C24 – H24A ···· O10	0.95	2.38	3.211(11)	145
C35 – H35A ···· O2 [iv]	0.95	2.51	3.357(11)	149
C38 – H38A ···· O11 [v]	0.95	2.44	3.049(17)	122
C43 – H43A ···· O2 [vi]	0.95	2.51	3.418(12)	160
O1W ····O1 [v]			3.026(17)	

symmetry: i = x,1+y,z; ii = 3/2-x,1/2+y,1/2-z; iii = 1/2-x,1/2+y,1/2-z; iv = 1-x,-1+y,1-z; v = 1/2-x,-1/2+y,1/2-z; vi = 1-x,y,1-z

$\{[Ag_3(4)_2](ClO_4)_3\}_n$

Table S7. Selected angles [°] of $\{[Ag_3(\mathbf{4})_2](ClO_4)_3\}_n$

angle	angle [°]	angle	angle [°]	angle	angle [°]
N(1) - Ag(1) - N(4)	75.99	N(7) - Ag(2) - N(11)	72.61	N(3) - Ag(3) - N(5)	121.00
N(1) - Ag(1) - N(6)	74.22	N(7) - Ag(2) - N(14)	147.60	N(3) - Ag(3) - N(9)	98.89
N(1) - Ag(1) - N(12)	145.21	N(8) - Ag(2) - N(10)	105.45	N(3) - Ag(3) - N(13)	115.57
N(4) - Ag(1) - N(6)	111.85	N(8) - Ag(2) - N(11)	106.88	N(5) - Ag(3) - N(9)	107.80
N(4) - Ag(1) - N(12)	129.35	N(8) - Ag(2) - N(14)	136.72	N(5) - Ag(3) - N(13)	108.62
N(6) - Ag(1) - N(12)	108.69	N(10) - Ag(2) - N(11)	120.55	N(9) - Ag(3) - N(13)	102.45
N(7) - Ag(2) - N(8)	73.92	N(10) - Ag(2) - N(14)	78.78		
N(7) - Ag(2) - N(10)	70.39	N(11) - Ag(2) - N(14)	100.60		

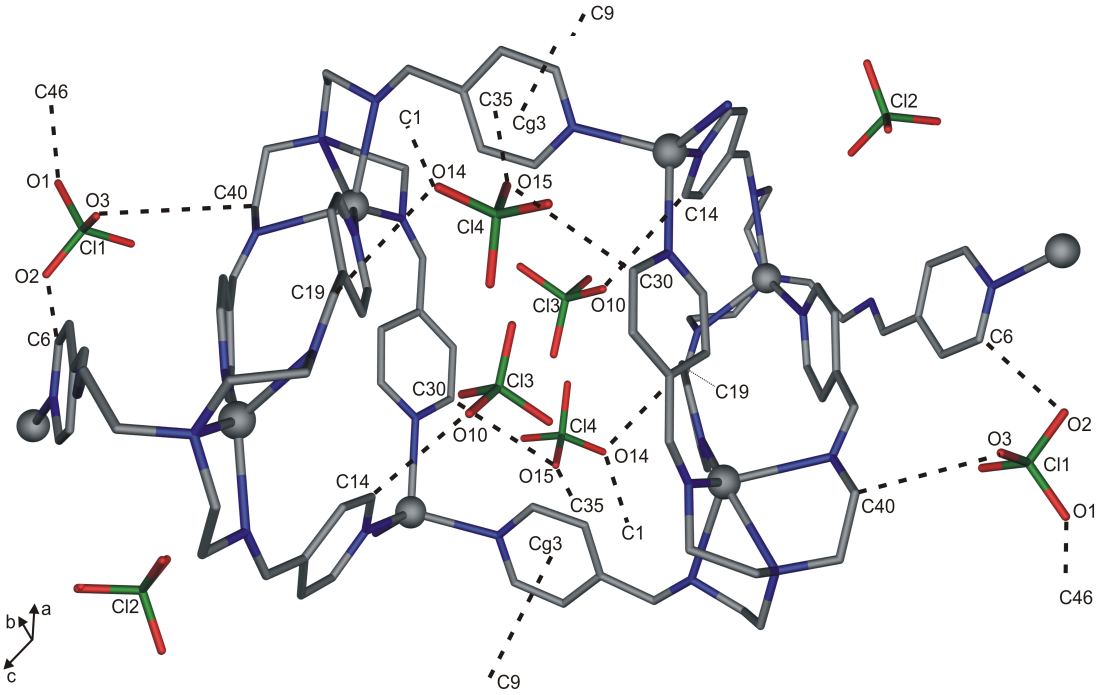

Fig. S5 Weak CH-O and π-π interactions in $\{[Ag_3(\mathbf{4})_2]ClO_4)_3\}_n$ as dashed lines, H atoms removed for clarity.

Table S8. Distance and angles of the CH-O interactions in $\{[Ag_3(\mathbf{4})_2]ClO_4)_3\}_n$

D-H	A	D-H [Å]	DH ··A [Å]	D···A [Å]	D-H-A [°]
C1-H1A	O14 [i]	0.99	2.34	3.108(8)	134
C6-H6A	O2	0.95	2.48	3.382(6)	158
C14-H14A	O10	0.95	2.23	3.174(9)	171
C19-H19A	O14	0.95	2.50	3.160(8)	126
C30-H30A	O15 [ii]	0.95	2.49	3.389(13)	157
C35-H35A	O15 [iii]	0.95	2.48	3.391(12)	160
C40-H40A	O3	0.99	2.45	3.397(7)	159
C46-H46A	O1 [iv]	0.95	2.52	3.470(5)	176

Symmetry transformation: (i) = 1-x,-y,2-z; (ii) = -x,-y,1-z; (iii) = 1-x,-y,1-z; (iv) = 1-x,1-y,2-z.