

Table 1. Crystal data and structure refinement for [Ag(tfa)(tpa)]_n.

Identification code	1	
Empirical formula	C ₁₇ H ₁₂ AgF ₃ N ₄ O ₂	
Formula weight	469.18	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.0840(16) Å	α = 90°.
	b = 21.921(4) Å	β = 94.952(4)°.
	c = 8.7269(17) Å	γ = 90°.
Volume	1731.3(6) Å ³	
Z	4	
Density (calculated)	1.800 Mg/m ³	
Absorption coefficient	1.215 mm ⁻¹	
F(000)	928	
Crystal size	.2 x .2 x .3 mm ³	
θ range for data collection	1.86 to 28.28°.	
Index ranges	-10 ≤ h ≤ 12, -28 ≤ k ≤ 29, -11 ≤ l ≤ 11	
Reflections collected	12471	
Independent reflections	4106 [R(int) = 0.0412]	
Completeness to θ = 28.28°	95.5 %	
Absorption correction	Empirical	
Max. and min. transmission	0.2950 and 0.2326	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4106 / 0 / 319	
Goodness-of-fit on F ²	0.778	
Final R indices [I > 2σ(I)]	R1 = 0.0293, wR2 = 0.0360	
R indices (all data)	R1 = 0.0810, wR2 = 0.0425	
Largest diff. peak and hole	0.307 and -0.377 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for [Ag(tfa)(tpa)]_n. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	1994(1)	5045(1)	9286(1)	55(1)
O(1)	1949(2)	3841(1)	9220(3)	92(1)
O(2)	-210(2)	4291(1)	9063(3)	81(1)
N(1)	1191(2)	5613(1)	7227(2)	43(1)
N(2)	5535(2)	6608(1)	6281(3)	52(1)
N(3)	6335(2)	4999(1)	8671(2)	45(1)
N(4)	3507(2)	6039(1)	6889(2)	41(1)
C(1)	1967(2)	6009(1)	6469(3)	39(1)
C(2)	1313(3)	6383(1)	5328(4)	52(1)
C(3)	-189(3)	6355(2)	4996(4)	59(1)
C(4)	-999(3)	5955(1)	5766(4)	56(1)
C(5)	-285(3)	5590(1)	6843(4)	52(1)
C(6)	4257(3)	6609(1)	6879(3)	39(1)
C(7)	3655(3)	7119(1)	7478(4)	60(1)
C(8)	4416(4)	7662(2)	7427(4)	71(1)
C(9)	5731(4)	7678(2)	6820(4)	66(1)
C(10)	6255(3)	7142(2)	6281(4)	66(1)
C(11)	5523(3)	5493(1)	8325(3)	41(1)
C(12)	4324(2)	5496(1)	7219(3)	36(1)
C(13)	3967(3)	4958(1)	6472(3)	47(1)
C(14)	4801(3)	4444(1)	6833(4)	56(1)
C(15)	5975(3)	4483(1)	7919(4)	52(1)

C(16)	609(3)	3857(1)	9227(3)	52(1)
C(17)	-111(5)	3240(2)	9479(6)	67(1)
F(1)	439(13)	2819(6)	8630(20)	107(5)
F(1A)	744(14)	2923(6)	10566(17)	139(4)
F(2)	17(12)	3058(6)	10894(16)	107(3)
F(2A)	-1368(10)	3253(6)	9952(12)	129(5)
F(3)	-1578(10)	3271(6)	9070(17)	153(6)
F(3A)	-213(13)	2881(6)	8301(17)	116(5)

Table 3. Bond lengths [Å] and angles [°] for [Ag(tfa)(tpa)]_n.

Ag(1)-N(3)#1	2.2417(19)
Ag(1)-N(1)	2.254(2)
Ag(1)-O(2)	2.590(2)
Ag(1)-O(1)	2.642(2)
Ag(1)-O(2)#2	2.687(2)
O(1)-C(16)	1.218(3)
O(2)-C(16)	1.210(3)
N(1)-C(1)	1.330(3)
N(1)-C(5)	1.355(3)
N(2)-C(6)	1.313(3)
N(2)-C(10)	1.339(3)
N(3)-C(11)	1.331(3)
N(3)-C(15)	1.334(3)
N(4)-C(1)	1.416(3)
N(4)-C(12)	1.420(3)
N(4)-C(6)	1.424(3)
C(1)-C(2)	1.383(3)
C(2)-C(3)	1.371(4)
C(3)-C(4)	1.360(4)
C(4)-C(5)	1.356(4)
C(6)-C(7)	1.368(3)
C(7)-C(8)	1.379(4)
C(8)-C(9)	1.348(4)
C(9)-C(10)	1.366(4)
C(11)-C(12)	1.392(3)
C(12)-C(13)	1.372(3)
C(13)-C(14)	1.379(4)
C(14)-C(15)	1.367(4)
C(16)-C(17)	1.527(4)
C(17)-F(2A)	1.247(8)
C(17)-F(3A)	1.291(13)
C(17)-F(2)	1.293(14)
C(17)-F(1)	1.305(14)
C(17)-F(3)	1.351(10)
C(17)-F(1A)	1.363(16)
N(3)#1-Ag(1)-N(1)	143.89(8)
N(3)#1-Ag(1)-O(2)	119.88(8)
N(1)-Ag(1)-O(2)	95.60(7)
C(16)-O(2)-Ag(1)	91.75(18)
C(1)-N(1)-C(5)	117.2(2)
C(1)-N(1)-Ag(1)	127.44(16)
C(5)-N(1)-Ag(1)	114.95(19)
C(6)-N(2)-C(10)	116.5(2)
C(11)-N(3)-C(15)	118.1(2)
C(11)-N(3)-Ag(1)#1	122.68(19)

C(15)-N(3)-Ag(1)#1	118.38(19)
C(1)-N(4)-C(12)	120.1(2)
C(1)-N(4)-C(6)	120.1(2)
C(12)-N(4)-C(6)	119.70(19)
N(1)-C(1)-C(2)	122.1(2)
N(1)-C(1)-N(4)	117.1(2)
C(2)-C(1)-N(4)	120.8(2)
C(3)-C(2)-C(1)	118.9(3)
C(4)-C(3)-C(2)	119.7(3)
C(5)-C(4)-C(3)	118.5(3)
N(1)-C(5)-C(4)	123.6(3)
N(2)-C(6)-C(7)	123.4(2)
N(2)-C(6)-N(4)	116.2(2)
C(7)-C(6)-N(4)	120.5(2)
C(6)-C(7)-C(8)	118.3(3)
C(9)-C(8)-C(7)	119.9(3)
C(8)-C(9)-C(10)	117.3(3)
N(2)-C(10)-C(9)	124.5(3)
N(3)-C(11)-C(12)	123.2(3)
C(13)-C(12)-C(11)	117.7(2)
C(13)-C(12)-N(4)	121.7(2)
C(11)-C(12)-N(4)	120.6(2)
C(12)-C(13)-C(14)	119.3(3)
C(15)-C(14)-C(13)	119.3(3)
N(3)-C(15)-C(14)	122.5(3)
O(2)-C(16)-O(1)	128.8(3)
O(2)-C(16)-C(17)	116.7(3)
O(1)-C(16)-C(17)	114.6(3)
F(2A)-C(17)-F(3A)	105.8(8)
F(2A)-C(17)-F(2)	72.6(7)
F(3A)-C(17)-F(2)	124.6(9)
F(2A)-C(17)-F(1)	127.5(8)
F(2)-C(17)-F(1)	108.3(10)
F(2)-C(17)-F(3)	105.9(8)
F(1)-C(17)-F(3)	107.7(8)
F(2A)-C(17)-F(1A)	105.3(8)
F(3A)-C(17)-F(1A)	104.0(9)
F(3)-C(17)-F(1A)	134.4(8)
F(2A)-C(17)-C(16)	116.3(7)
F(3A)-C(17)-C(16)	115.3(8)
F(2)-C(17)-C(16)	113.9(6)
F(1)-C(17)-C(16)	110.8(7)
F(3)-C(17)-C(16)	110.0(6)
F(1A)-C(17)-C(16)	109.1(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2 #2 -x,-y+1,-z+2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{tfa})(\text{tpa})]_n$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	46(1)	52(1)	66(1)	17(1)	-3(1)	-1(1)
O(1)	51(1)	77(2)	148(2)	-1(2)	8(1)	-8(1)
O(2)	88(2)	56(2)	103(2)	15(1)	30(1)	24(1)
N(1)	34(1)	38(1)	56(2)	7(1)	-1(1)	-6(1)
N(2)	40(1)	41(2)	77(2)	-5(1)	14(1)	-6(1)

N(3)	41(1)	37(1)	57(1)	4(2)	4(1)	8(1)
N(4)	30(1)	29(1)	65(2)	10(1)	-1(1)	-1(1)
C(1)	35(1)	34(2)	48(2)	-3(1)	0(1)	2(1)
C(2)	43(2)	53(2)	59(2)	17(2)	7(2)	-3(2)
C(3)	51(2)	61(2)	60(2)	13(2)	-16(2)	11(2)
C(4)	33(2)	56(2)	75(2)	1(2)	-13(2)	-1(2)
C(5)	36(2)	53(2)	67(2)	6(2)	0(2)	-9(2)
C(6)	35(1)	30(2)	51(2)	5(1)	1(1)	1(1)
C(7)	49(2)	44(2)	91(3)	-7(2)	27(2)	-4(2)
C(8)	70(2)	40(2)	106(3)	-13(2)	23(2)	-2(2)
C(9)	62(2)	40(2)	97(3)	2(2)	9(2)	-18(2)
C(10)	48(2)	53(2)	101(3)	-2(2)	25(2)	-11(2)
C(11)	42(2)	31(2)	52(2)	-2(2)	6(2)	-5(1)
C(12)	31(1)	33(2)	45(2)	6(1)	4(1)	0(1)
C(13)	48(1)	42(2)	51(2)	-3(2)	-5(1)	0(2)
C(14)	63(2)	35(2)	68(3)	-13(2)	-4(2)	2(2)
C(15)	55(2)	35(2)	66(2)	3(2)	2(2)	15(2)
C(16)	60(2)	42(2)	57(2)	-2(2)	11(2)	0(2)
C(17)	81(3)	52(3)	69(3)	4(2)	9(3)	-7(2)
F(1)	118(7)	35(4)	171(14)	-24(5)	38(7)	-4(5)
F(1A)	206(12)	81(5)	126(11)	54(6)	2(8)	5(6)
F(2)	145(10)	97(7)	81(6)	25(4)	19(6)	-31(6)
F(2A)	96(8)	146(7)	156(10)	-8(7)	77(8)	-53(7)
F(3)	67(5)	93(5)	286(15)	38(9)	-66(8)	-29(4)
F(3A)	172(13)	97(9)	82(5)	-43(5)	28(8)	-76(9)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $[\text{Ag}(\text{tfa})(\text{tpa})]_n$.

	x	y	z	U(eq)
H(2)	1870(20)	6614(9)	4800(20)	32(7)
H(3)	-570(20)	6591(10)	4250(30)	45(8)
H(4)	-2080(20)	5950(10)	5630(30)	51(7)
H(5)	-790(20)	5306(9)	7430(20)	37(7)
H(7)	2810(20)	7119(10)	7880(30)	39(8)
H(8)	4090(30)	7992(11)	7890(30)	59(9)
H(9)	6270(30)	8017(11)	6740(30)	62(9)
H(10)	7140(30)	7107(11)	5850(30)	64(9)
H(11)	5790(20)	5812(9)	8850(20)	23(7)
H(13)	3140(20)	4939(9)	5700(20)	42(6)
H(14)	4610(20)	4090(10)	6370(30)	48(8)
H(15)	6580(30)	4163(11)	8210(30)	64(9)

Table 1. Crystal data and structure refinement for $[\text{Ag}(\text{NO}_3)(\text{tpa})(\text{MeCN})]_n$.

Identification code	2	
Empirical formula	$\text{C}_{17}\text{H}_{15}\text{AgN}_6\text{O}_3$	
Formula weight	459.22	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	$a = 13.334(4)$ Å	$\alpha = 90^\circ$.
	$b = 15.668(4)$ Å	$\beta = 106.232(5)^\circ$.
	$c = 9.031(2)$ Å	$\gamma = 90^\circ$.
Volume	$1811.7(8)$ Å ³	
Z	4	
Density (calculated)	1.684 Mg/m ³	
Absorption coefficient	1.144 mm ⁻¹	
F(000)	920	
Crystal size	.1 x .3 x .4 mm ³	
θ range for data collection	2.05 to 28.32°	
Index ranges	-17 ≤ h ≤ 17, -20 ≤ k ≤ 20, -10 ≤ l ≤ 12	
Reflections collected	12899	
Independent reflections	4297 [R(int) = 0.0329]	
Completeness to $\theta = 28.32^\circ$	95.4 %	
Absorption correction	Empirical	
Max. and min. transmission	0.3484 and 0.2946	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4297 / 0 / 244	
Goodness-of-fit on F ²	0.831	
Final R indices [I > 2σ(I)]	R1 = 0.0296, wR2 = 0.0519	
R indices (all data)	R1 = 0.0732, wR2 = 0.0597	
Largest diff. peak and hole	0.410 and -0.428 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² × 10³) for $[\text{Ag}(\text{NO}_3)(\text{tpa})(\text{MeCN})]_n$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	2520(1)	209(1)	8498(1)	61(1)
O(1)	3599(2)	-915(2)	10386(3)	93(1)
O(2)	2280(2)	-1443(2)	8808(3)	102(1)
O(3)	3176(2)	-2198(2)	10653(3)	110(1)
N(1)	2817(2)	55(1)	6131(2)	41(1)
N(2)	1192(2)	2278(1)	6294(2)	57(1)
N(3)	3388(2)	3681(1)	5004(2)	51(1)
N(4)	2552(2)	1517(1)	5701(2)	42(1)
N(5)	3027(2)	-1536(2)	9951(3)	60(1)
N(6)	795(2)	516(2)	8615(3)	77(1)
C(1)	2924(2)	730(2)	5292(3)	38(1)
C(2)	3379(2)	676(2)	4095(3)	55(1)
C(3)	3718(2)	-102(2)	3738(3)	63(1)
C(4)	3594(2)	-806(2)	4563(3)	58(1)
C(5)	3134(2)	-706(2)	5743(3)	47(1)
C(6)	1471(2)	1616(2)	5532(3)	40(1)
C(7)	772(2)	1073(2)	4619(3)	42(1)
C(8)	-260(2)	1217(2)	4436(3)	64(1)
C(9)	-588(2)	1898(2)	5148(4)	67(1)
C(10)	149(3)	2402(2)	6067(3)	62(1)
C(11)	2818(2)	2983(2)	4976(3)	45(1)
C(12)	3193(2)	2246(2)	5782(3)	39(1)

C(13)	4231(2)	2236(2)	6642(3)	49(1)
C(14)	4829(2)	2946(2)	6632(3)	56(1)
C(15)	4393(2)	3653(2)	5818(3)	54(1)
C(16)	-38(3)	676(2)	8495(3)	64(1)
C(17)	-1123(3)	897(3)	8345(4)	101(1)

Table 3. Bond lengths [Å] and angles [°] for [Ag(NO₃)(tpa)(MeCN)]_n.

Ag(1)-N(1)	2.294(2)
Ag(1)-N(3)#1	2.310(2)
Ag(1)-N(6)	2.381(3)
Ag(1)-O(1)	2.590(3)
O(1)-N(5)	1.231(3)
O(2)-N(5)	1.226(3)
O(3)-N(5)	1.204(3)
N(1)-C(1)	1.330(3)
N(1)-C(5)	1.344(3)
N(2)-C(6)	1.354(3)
N(2)-C(10)	1.363(3)
N(3)-C(11)	1.327(3)
N(3)-C(15)	1.336(3)
N(3)-Ag(1)#2	2.310(2)
N(4)-C(6)	1.415(3)
N(4)-C(1)	1.416(3)
N(4)-C(12)	1.417(3)
N(6)-C(16)	1.114(4)
C(1)-C(2)	1.383(3)
C(2)-C(3)	1.368(4)
C(3)-C(4)	1.367(4)
C(4)-C(5)	1.379(3)
C(6)-C(7)	1.357(3)
C(7)-C(8)	1.359(4)
C(8)-C(9)	1.378(4)
C(9)-C(10)	1.350(4)
C(11)-C(12)	1.383(3)
C(12)-C(13)	1.385(3)
C(13)-C(14)	1.371(3)
C(14)-C(15)	1.367(4)
C(16)-C(17)	1.458(5)

N(1)-Ag(1)-N(3)#1	116.08(7)
N(1)-Ag(1)-N(6)	118.90(9)
N(3)#1-Ag(1)-N(6)	98.83(9)
N(1)-Ag(1)-O(1)	109.43(7)
N(3)#1-Ag(1)-O(1)	91.72(8)
N(6)-Ag(1)-O(1)	118.30(9)
N(5)-O(1)-Ag(1)	98.4(2)
C(1)-N(1)-C(5)	117.7(2)
C(1)-N(1)-Ag(1)	121.36(16)
C(5)-N(1)-Ag(1)	119.02(16)
C(6)-N(2)-C(10)	116.5(2)
C(11)-N(3)-C(15)	117.7(2)
C(11)-N(3)-Ag(1)#2	114.73(19)
C(15)-N(3)-Ag(1)#2	127.48(18)
C(6)-N(4)-C(1)	119.2(2)
C(6)-N(4)-C(12)	120.0(2)
C(1)-N(4)-C(12)	117.7(2)

O(3)-N(5)-O(2)	121.4(3)
O(3)-N(5)-O(1)	121.1(3)
O(2)-N(5)-O(1)	117.4(3)
C(16)-N(6)-Ag(1)	172.1(3)
N(1)-C(1)-C(2)	122.4(2)
N(1)-C(1)-N(4)	116.3(2)
C(2)-C(1)-N(4)	121.3(2)
C(3)-C(2)-C(1)	119.0(3)
C(4)-C(3)-C(2)	119.5(3)
C(3)-C(4)-C(5)	118.5(3)
N(1)-C(5)-C(4)	122.8(3)
N(2)-C(6)-C(7)	123.4(3)
N(2)-C(6)-N(4)	116.5(2)
C(7)-C(6)-N(4)	120.2(2)
C(6)-C(7)-C(8)	118.0(3)
C(7)-C(8)-C(9)	121.0(3)
C(10)-C(9)-C(8)	118.0(3)
C(9)-C(10)-N(2)	123.1(3)
N(3)-C(11)-C(12)	123.8(3)
C(11)-C(12)-C(13)	117.5(2)
C(11)-C(12)-N(4)	121.5(2)
C(13)-C(12)-N(4)	120.9(2)
C(14)-C(13)-C(12)	118.7(3)
C(15)-C(14)-C(13)	120.0(3)
N(3)-C(15)-C(14)	122.2(3)
N(6)-C(16)-C(17)	179.2(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2 #2 x,-y+1/2,z-1/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{NO}_3)(\text{tpa})(\text{MeCN})]_n$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	89(1)	39(1)	61(1)	-2(1)	30(1)	2(1)
O(1)	108(2)	71(2)	107(2)	-18(2)	43(2)	-19(2)
O(2)	89(2)	121(2)	81(2)	27(2)	0(2)	-3(2)
O(3)	112(2)	68(2)	145(2)	59(2)	27(2)	19(2)
N(1)	43(1)	33(1)	47(1)	1(1)	12(1)	4(1)
N(2)	62(2)	48(2)	64(1)	-1(1)	22(1)	4(1)
N(3)	59(2)	37(1)	56(1)	6(1)	17(1)	-10(1)
N(4)	39(1)	30(1)	57(1)	1(1)	13(1)	0(1)
N(5)	66(2)	52(2)	70(2)	10(2)	32(2)	11(2)
N(6)	69(2)	78(2)	92(2)	5(2)	37(2)	4(2)
C(1)	35(2)	32(1)	46(1)	0(1)	9(1)	-1(1)
C(2)	64(2)	50(2)	57(2)	-1(2)	27(2)	-7(2)
C(3)	68(2)	65(2)	67(2)	-14(2)	36(2)	-9(2)
C(4)	52(2)	51(2)	75(2)	-18(2)	23(2)	3(2)
C(5)	44(2)	33(2)	60(2)	0(1)	9(1)	3(1)
C(6)	41(2)	32(2)	47(1)	8(1)	14(1)	3(1)
C(7)	40(2)	33(1)	52(2)	-5(1)	10(1)	2(1)
C(8)	56(2)	56(2)	70(2)	2(2)	2(2)	-12(2)
C(9)	41(2)	66(2)	93(2)	17(2)	19(2)	4(2)
C(10)	63(2)	50(2)	84(2)	0(2)	37(2)	11(2)
C(11)	44(2)	41(2)	46(1)	4(1)	3(1)	-4(1)
C(12)	42(2)	33(1)	42(1)	0(1)	11(1)	-3(1)
C(13)	43(2)	45(2)	56(2)	5(1)	10(2)	5(2)

C(14)	36(2)	59(2)	68(2)	-6(2)	8(2)	-5(2)
C(15)	54(2)	45(2)	68(2)	-7(2)	23(2)	-16(2)
C(16)	65(3)	72(2)	58(2)	-1(2)	21(2)	-9(2)
C(17)	57(3)	150(4)	95(3)	17(3)	20(2)	1(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $[\text{Ag}(\text{NO}_3)(\text{tpa})(\text{MeCN})]_n$.

	x	y	z	U(eq)
H(2)	3453	1160	3540	66
H(3)	4031	-150	2942	76
H(4)	3815	-1340	4333	70
H(5)	3038	-1186	6293	56
H(7)	993	615	4134	51
H(8)	-753	851	3821	77
H(9)	-1295	2007	5000	80
H(10)	-66	2855	6570	75
H(11)	2125	2991	4380	54
H(13)	4516	1757	7215	58
H(14)	5533	2946	7179	67
H(15)	4808	4131	5831	65
H(17A)	-1251	872	9339	151
H(17B)	-1575	502	7659	151
H(17C)	-1260	1465	7937	151

Table 1. Crystal data and structure refinement for [Ag(OTf)(tpa)]_n.

Identification code	3	
Empirical formula	C ₁₆ H ₁₂ AgF ₃ N ₄ O ₃ S	
Formula weight	505.23	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.978(4) Å	α = 90°.
	b = 26.051(10) Å	β = 100.546(7)°.
	c = 6.444(2) Å	γ = 90°.
Volume	1811.7(11) Å ³	
Z	4	
Density (calculated)	1.852 Mg/m ³	
Absorption coefficient	1.284 mm ⁻¹	
F(000)	1000	
Crystal size	.1 x .1 x .4 mm ³	
Theta range for data collection	1.89 to 28.38°.	
Index ranges	-14 ≤ h ≤ 14, -34 ≤ k ≤ 34, -8 ≤ l ≤ 7	
Reflections collected	12861	
Independent reflections	4138 [R(int) = 0.1157]	
Completeness to theta = 28.38°	90.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.3169 and 0.2531	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4138 / 0 / 249	
Goodness-of-fit on F ²	0.893	
Final R indices [I > 2σ(I)]	R1 = 0.1271, wR2 = 0.3012	
R indices (all data)	R1 = 0.2644, wR2 = 0.3613	
Largest diff. peak and hole	5.300 and -0.764 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for [Ag(OTf)(tpa)]_n. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	4702(1)	3406(1)	8335(2)	48(1)
O(1)	3006(11)	4006(5)	8905(19)	57(3)
O(2)	1246(13)	3431(5)	8100(20)	67(4)
O(3)	1667(12)	4037(5)	5513(17)	56(3)
S(1)	1780(4)	3917(2)	7677(7)	45(1)
F(1)	927(14)	4342(6)	10760(20)	104(5)
F(2)	-336(12)	4349(6)	7860(20)	107(5)
F(3)	1241(13)	4857(5)	8400(20)	94(4)
N(1)	5580(12)	4076(5)	6810(20)	39(3)
N(2)	6788(13)	3339(6)	950(20)	48(4)
N(3)	4263(13)	2432(5)	3438(19)	34(3)
N(4)	6065(13)	3616(5)	3960(20)	43(4)
C(1)	6098(17)	4079(6)	5150(30)	45(4)
C(2)	6791(17)	4494(7)	4640(30)	51(5)
C(3)	6879(18)	4925(7)	5880(30)	60(5)
C(4)	6308(18)	4940(7)	7570(30)	58(5)
C(5)	5660(17)	4495(6)	7960(30)	47(5)
C(6)	7060(15)	3474(6)	2950(30)	38(4)
C(7)	8277(18)	3476(9)	4060(30)	66(6)
C(8)	9228(19)	3340(10)	3020(40)	83(8)
C(9)	8920(20)	3205(10)	910(40)	86(8)
C(10)	7720(20)	3204(8)	0(30)	61(6)

C(11)	5161(15)	2771(7)	3750(20)	39(4)
C(12)	4924(14)	3331(6)	3700(20)	30(3)
C(13)	3816(16)	3475(7)	3280(20)	43(4)
C(14)	2848(16)	3121(7)	3040(30)	45(4)
C(15)	3108(15)	2602(6)	3100(20)	37(4)
C(16)	870(20)	4402(9)	8710(40)	66(6)

Table 3. Bond lengths [Å] and angles [°] for [Ag(OTf)(tpa)]_n.

Ag(1)-N(3)#1	2.238(13)
Ag(1)-N(1)	2.299(13)
Ag(1)-O(1)	2.509(12)
Ag(1)-N(2)#2	2.588(15)
O(1)-S(1)	1.450(12)
O(2)-S(1)	1.443(13)
O(3)-S(1)	1.413(12)
S(1)-C(16)	1.81(2)
F(1)-C(16)	1.32(2)
F(2)-C(16)	1.34(2)
F(3)-C(16)	1.28(2)
N(1)-C(1)	1.300(19)
N(1)-C(5)	1.313(19)
N(2)-C(6)	1.32(2)
N(2)-C(10)	1.33(2)
N(2)-Ag(1)#3	2.588(15)
N(3)-C(11)	1.31(2)
N(3)-C(15)	1.324(19)
N(3)-Ag(1)#4	2.238(13)
N(4)-C(1)	1.42(2)
N(4)-C(6)	1.42(2)
N(4)-C(12)	1.44(2)
C(1)-C(2)	1.39(2)
C(2)-C(3)	1.37(2)
C(3)-C(4)	1.35(2)
C(4)-C(5)	1.41(2)
C(6)-C(7)	1.40(2)
C(7)-C(8)	1.39(3)
C(8)-C(9)	1.38(3)
C(9)-C(10)	1.34(3)
C(11)-C(12)	1.48(2)
C(12)-C(13)	1.25(2)
C(13)-C(14)	1.39(2)
C(14)-C(15)	1.38(2)
N(3)#1-Ag(1)-N(1)	149.6(4)
N(3)#1-Ag(1)-O(1)	115.7(5)
N(1)-Ag(1)-O(1)	88.2(4)
N(3)#1-Ag(1)-N(2)#2	94.8(5)
N(1)-Ag(1)-N(2)#2	86.5(5)
O(1)-Ag(1)-N(2)#2	122.6(4)
S(1)-O(1)-Ag(1)	117.4(7)
O(3)-S(1)-O(2)	114.7(8)
O(3)-S(1)-O(1)	114.1(8)
O(2)-S(1)-O(1)	113.9(8)
O(3)-S(1)-C(16)	104.6(10)
O(2)-S(1)-C(16)	105.7(10)
O(1)-S(1)-C(16)	102.1(9)

C(1)-N(1)-C(5)	117.8(15)
C(1)-N(1)-Ag(1)	129.4(11)
C(5)-N(1)-Ag(1)	112.4(11)
C(6)-N(2)-C(10)	117.5(16)
C(6)-N(2)-Ag(1)#3	129.3(11)
C(10)-N(2)-Ag(1)#3	112.7(12)
C(11)-N(3)-C(15)	118.0(14)
C(11)-N(3)-Ag(1)#4	120.1(11)
C(15)-N(3)-Ag(1)#4	121.8(11)
C(1)-N(4)-C(6)	121.5(14)
C(1)-N(4)-C(12)	115.9(14)
C(6)-N(4)-C(12)	122.3(13)
N(1)-C(1)-C(2)	122.5(16)
N(1)-C(1)-N(4)	117.8(15)
C(2)-C(1)-N(4)	119.3(16)
C(3)-C(2)-C(1)	118.8(17)
C(4)-C(3)-C(2)	119.8(17)
C(3)-C(4)-C(5)	116.4(17)
N(1)-C(5)-C(4)	124.6(17)
N(2)-C(6)-C(7)	121.8(15)
N(2)-C(6)-N(4)	117.8(15)
C(7)-C(6)-N(4)	120.4(15)
C(8)-C(7)-C(6)	119.1(19)
C(9)-C(8)-C(7)	118(2)
C(10)-C(9)-C(8)	118(2)
N(2)-C(10)-C(9)	125.3(19)
N(3)-C(11)-C(12)	122.4(15)
C(13)-C(12)-N(4)	131.3(16)
C(13)-C(12)-C(11)	117.3(15)
N(4)-C(12)-C(11)	111.1(13)
C(12)-C(13)-C(14)	121.0(17)
C(15)-C(14)-C(13)	119.7(17)
N(3)-C(15)-C(14)	121.4(15)
F(3)-C(16)-F(1)	107.6(18)
F(3)-C(16)-F(2)	111(2)
F(1)-C(16)-F(2)	105.3(19)
F(3)-C(16)-S(1)	111.9(16)
F(1)-C(16)-S(1)	110.7(16)
F(2)-C(16)-S(1)	110.3(14)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z+1/2 #2 x,y,z+1 #3 x,y,z-1 #4 x,-y+1/2,z-1/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{OTf})(\text{tpa})]_n$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	49(1)	32(1)	63(1)	2(1)	12(1)	-2(1)
O(1)	38(7)	57(9)	74(8)	-11(7)	5(7)	5(6)
O(2)	70(9)	37(8)	94(10)	5(7)	17(8)	-3(7)
O(3)	63(9)	60(9)	45(7)	-1(6)	11(6)	-11(7)
S(1)	43(3)	36(3)	56(3)	-2(2)	13(2)	4(2)
F(1)	115(12)	130(14)	74(9)	-29(9)	37(8)	14(10)
F(2)	52(8)	105(12)	158(14)	-50(10)	3(9)	14(8)
F(3)	97(10)	43(8)	136(12)	-14(8)	8(9)	8(7)
N(1)	44(9)	31(8)	45(8)	-12(7)	13(7)	-6(6)

N(2)	42(9)	57(11)	50(9)	-7(7)	20(7)	-12(7)
N(3)	32(8)	29(7)	42(7)	-5(6)	7(6)	-1(6)
N(4)	52(10)	33(8)	49(8)	-12(7)	21(7)	-7(7)
C(1)	58(12)	26(9)	48(10)	-5(8)	7(9)	-6(8)
C(2)	50(12)	50(12)	58(11)	0(9)	21(10)	-11(9)
C(3)	61(13)	25(10)	96(15)	-6(10)	17(12)	-17(9)
C(4)	62(13)	33(11)	82(14)	-19(10)	20(11)	-8(9)
C(5)	54(12)	26(9)	60(11)	-14(9)	7(9)	-2(8)
C(6)	36(10)	34(10)	48(10)	-10(8)	18(8)	-6(7)
C(7)	42(12)	88(18)	69(13)	-18(12)	13(10)	-4(11)
C(8)	30(11)	130(20)	95(17)	-37(16)	22(11)	-13(13)
C(9)	69(18)	100(20)	97(19)	-46(15)	43(15)	-25(14)
C(10)	59(15)	78(16)	52(11)	-20(10)	22(11)	-8(11)
C(11)	32(9)	53(12)	33(8)	-2(8)	7(7)	3(8)
C(13)	51(11)	33(10)	40(9)	-1(8)	-7(8)	-8(8)
C(14)	37(10)	50(12)	51(10)	3(9)	14(8)	3(9)
C(15)	29(9)	36(10)	42(9)	-10(8)	0(7)	-15(7)
C(16)	63(16)	58(15)	76(15)	-21(12)	12(12)	-6(11)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{OTf})(\text{tpa})]_n$.

	x	y	z	U(eq)
H(2)	7186	4478	3486	62
H(3)	7329	5207	5555	72
H(4)	6343	5228	8431	70
H(5)	5261	4498	9118	56
H(7)	8447	3567	5475	79
H(8)	10048	3341	3714	100
H(9)	9533	3117	148	103
H(10)	7526	3101	-1401	74
H(11)	5977	2656	4009	47
H(13)	3638	3823	3123	52
H(14)	2031	3233	2843	54
H(15)	2458	2368	2892	44

Table 1. Crystal data and structure refinement for $[\text{Ag}(\text{PF}_6)(\text{tpa})(\text{MeCN})]_n$.

Identification code	4	
Empirical formula	$\text{C}_{17}\text{H}_{15}\text{AgF}_6\text{N}_5\text{P}$	
Formula weight	542.18	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	$a = 6.4389(14)$ Å	$\alpha = 90^\circ$
	$b = 23.574(5)$ Å	$\beta = 90^\circ$
	$c = 25.400(5)$ Å	$\gamma = 90^\circ$
Volume	$3855.5(14)$ Å ³	
Z	8	
Density (calculated)	1.868 Mg/m ³	
Absorption coefficient	1.200 mm ⁻¹	
F(000)	2144	
Crystal size	.4 x .4 x .4 mm ³	
Theta range for data collection	1.73 to 28.29°	
Index ranges	-8 ≤ h ≤ 8, -31 ≤ k ≤ 31, -33 ≤ l ≤ 31	
Reflections collected	25738	
Independent reflections	4637 [R(int) = 0.0676]	
Completeness to theta = 28.29°	96.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.3069 and 0.2000	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4637 / 0 / 271	
Goodness-of-fit on F ²	1.444	
Final R indices [I > 2σ(I)]	R1 = 0.0553, wR2 = 0.1952	
R indices (all data)	R1 = 0.0712, wR2 = 0.2062	
Largest diff. peak and hole	2.204 and -1.441 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å² × 10³) for $[\text{Ag}(\text{PF}_6)(\text{tpa})(\text{MeCN})]_n$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	3712(1)	3727(1)	1692(1)	64(1)
P(1)	1416(2)	1020(1)	1318(1)	58(1)
F(1)	1736(7)	1183(2)	717(2)	114(2)
F(2)	1066(7)	873(2)	1917(2)	109(1)
F(3)	1409(8)	1664(2)	1453(2)	122(2)
F(4)	-987(6)	1028(3)	1225(2)	121(2)
F(5)	1410(10)	379(2)	1188(3)	176(3)
F(6)	3823(6)	1007(4)	1391(3)	148(2)
N(1)	2213(5)	4073(1)	909(1)	44(1)
N(2)	-4008(5)	3143(2)	1220(1)	50(1)
N(3)	-1614(4)	4128(1)	2522(1)	39(1)
N(4)	-1170(5)	3757(1)	1116(1)	43(1)
N(5)	2034(11)	2778(2)	2155(3)	98(2)
C(1)	272(6)	3972(2)	740(1)	39(1)
C(2)	-328(7)	4060(2)	226(1)	52(1)
C(3)	1106(7)	4257(2)	-137(2)	58(1)
C(4)	3087(8)	4373(2)	45(2)	57(1)
C(5)	3558(6)	4280(2)	557(2)	56(1)
C(6)	-2114(6)	3237(2)	1019(1)	41(1)
C(7)	-1092(7)	2831(2)	712(2)	60(1)
C(8)	-2090(11)	2333(2)	598(2)	78(2)
C(9)	-4051(10)	2241(2)	791(2)	80(2)

C(10)	-4920(9)	2641(2)	1103(2)	67(1)
C(11)	-1453(5)	3832(2)	2075(2)	39(1)
C(12)	-1468(5)	4085(2)	1583(1)	37(1)
C(13)	-1633(6)	4672(2)	1559(2)	47(1)
C(14)	-1803(7)	4976(2)	2018(2)	52(1)
C(15)	-1770(6)	4695(2)	2489(2)	47(1)
C(16)	1946(14)	2393(3)	2416(3)	98(2)
C(17)	1920(20)	1902(4)	2774(4)	159(5)

Table 3. Bond lengths [Å] and angles [°] for [Ag(PF₆)(tpa)(MeCN)]_n.

Ag(1)-N(3)#1	2.218(3)
Ag(1)-N(2)#2	2.342(4)
Ag(1)-N(1)	2.356(3)
P(1)-F(4)	1.566(4)
P(1)-F(5)	1.547(5)
P(1)-F(3)	1.555(4)
P(1)-F(1)	1.586(4)
P(1)-F(2)	1.578(4)
P(1)-F(6)	1.561(4)
N(1)-C(5)	1.337(5)
N(1)-C(1)	1.343(5)
N(2)-C(6)	1.341(5)
N(2)-C(10)	1.356(6)
N(2)-Ag(1)#3	2.342(4)
N(3)-C(11)	1.339(5)
N(3)-C(15)	1.343(5)
N(3)-Ag(1)#4	2.218(3)
N(4)-C(6)	1.391(5)
N(4)-C(1)	1.426(4)
N(4)-C(12)	1.428(5)
N(5)-C(16)	1.127(8)
C(1)-C(2)	1.377(5)
C(2)-C(3)	1.385(6)
C(3)-C(4)	1.384(6)
C(4)-C(5)	1.353(7)
C(6)-C(7)	1.397(6)
C(7)-C(8)	1.370(7)
C(8)-C(9)	1.371(9)
C(9)-C(10)	1.352(8)
C(11)-C(12)	1.384(5)
C(12)-C(13)	1.391(6)
C(13)-C(14)	1.373(6)
C(14)-C(15)	1.369(6)
C(16)-C(17)	1.473(11)
N(3)#1-Ag(1)-N(2)#2	140.36(12)
N(3)#1-Ag(1)-N(1)	124.97(11)
N(2)#2-Ag(1)-N(1)	91.63(12)
F(4)-P(1)-F(5)	88.7(4)
F(4)-P(1)-F(3)	91.1(3)
F(5)-P(1)-F(3)	179.4(4)
F(4)-P(1)-F(1)	88.9(3)
F(5)-P(1)-F(1)	91.8(3)
F(3)-P(1)-F(1)	88.7(3)
F(4)-P(1)-F(2)	90.4(2)
F(5)-P(1)-F(2)	89.4(3)

F(3)-P(1)-F(2)	90.1(2)
F(1)-P(1)-F(2)	178.6(3)
F(4)-P(1)-F(6)	178.2(4)
F(5)-P(1)-F(6)	90.5(4)
F(3)-P(1)-F(6)	89.8(4)
F(1)-P(1)-F(6)	89.5(3)
F(2)-P(1)-F(6)	91.2(3)
C(5)-N(1)-C(1)	116.9(3)
C(5)-N(1)-Ag(1)	115.2(3)
C(1)-N(1)-Ag(1)	126.2(2)
C(6)-N(2)-C(10)	116.9(4)
C(6)-N(2)-Ag(1)#3	132.0(3)
C(10)-N(2)-Ag(1)#3	110.8(3)
C(11)-N(3)-C(15)	118.2(3)
C(11)-N(3)-Ag(1)#4	122.3(3)
C(15)-N(3)-Ag(1)#4	119.2(2)
C(6)-N(4)-C(1)	118.6(3)
C(6)-N(4)-C(12)	124.5(3)
C(1)-N(4)-C(12)	116.9(3)
N(1)-C(1)-C(2)	122.5(3)
N(1)-C(1)-N(4)	117.0(3)
C(2)-C(1)-N(4)	120.5(4)
C(3)-C(2)-C(1)	119.6(4)
C(4)-C(3)-C(2)	117.3(4)
C(3)-C(4)-C(5)	119.7(4)
N(1)-C(5)-C(4)	123.8(4)
N(2)-C(6)-C(7)	122.0(4)
N(2)-C(6)-N(4)	118.2(3)
C(7)-C(6)-N(4)	119.8(4)
C(6)-C(7)-C(8)	118.9(5)
C(9)-C(8)-C(7)	119.5(5)
C(10)-C(9)-C(8)	118.7(5)
C(9)-C(10)-N(2)	123.9(5)
N(3)-C(11)-C(12)	122.7(4)
C(11)-C(12)-C(13)	118.1(4)
C(11)-C(12)-N(4)	121.0(3)
C(13)-C(12)-N(4)	120.8(3)
C(14)-C(13)-C(12)	119.1(4)
C(13)-C(14)-C(15)	119.4(4)
N(3)-C(15)-C(14)	122.5(4)
N(5)-C(16)-C(17)	176.9(10)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, y, -z+1/2$ #2 $x+1, y, z$ #3 $x-1, y, z$ #4 $x-1/2, y, -z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{PF}_6)(\text{tpa})(\text{MeCN})]_n$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	58(1)	98(1)	35(1)	-6(1)	1(1)	-1(1)
P(1)	64(1)	59(1)	50(1)	-1(1)	2(1)	-8(1)
F(1)	115(3)	175(5)	54(2)	-5(2)	21(2)	-29(3)
F(2)	167(4)	93(3)	65(2)	21(2)	-5(2)	-20(2)
F(3)	210(6)	60(2)	94(3)	0(2)	13(3)	-23(2)
F(4)	68(2)	191(5)	103(3)	22(3)	4(2)	-23(3)
F(5)	276(9)	75(3)	176(6)	-45(3)	4(4)	10(3)

F(6)	71(3)	226(7)	147(5)	24(5)	-16(3)	7(3)
N(1)	41(2)	57(2)	35(1)	-2(1)	0(1)	-3(2)
N(2)	51(2)	54(2)	45(2)	2(1)	2(1)	-11(2)
N(3)	34(2)	55(2)	30(1)	-3(1)	-1(1)	0(1)
N(4)	47(2)	49(2)	31(2)	-2(1)	5(1)	-11(1)
N(5)	109(4)	73(3)	114(4)	2(3)	5(4)	-1(3)
C(1)	42(2)	44(2)	33(2)	-1(1)	2(1)	-5(2)
C(2)	52(2)	70(3)	35(2)	0(2)	-5(2)	-10(2)
C(3)	74(3)	69(3)	32(2)	3(2)	2(2)	-10(2)
C(4)	64(3)	59(3)	48(2)	2(2)	20(2)	-15(2)
C(5)	44(2)	72(3)	51(2)	-5(2)	7(2)	-14(2)
C(6)	48(2)	43(2)	32(2)	2(1)	-3(2)	-4(2)
C(7)	68(3)	51(2)	61(3)	-5(2)	10(2)	-3(2)
C(8)	111(5)	50(3)	74(3)	-16(2)	13(3)	0(3)
C(9)	110(5)	56(3)	72(3)	-11(2)	9(3)	-26(3)
C(10)	67(3)	73(3)	60(2)	-2(2)	4(2)	-29(3)
C(11)	34(2)	45(2)	37(2)	0(1)	0(1)	0(1)
C(12)	36(2)	42(2)	33(2)	-4(1)	-1(1)	-2(1)
C(13)	48(2)	47(2)	45(2)	9(2)	2(2)	0(2)
C(14)	52(2)	45(2)	58(2)	-5(2)	3(2)	5(2)
C(15)	37(2)	59(2)	45(2)	-15(2)	0(2)	3(2)
C(16)	142(6)	72(4)	81(4)	-10(3)	12(4)	-7(4)
C(17)	249(14)	119(7)	110(7)	26(5)	38(8)	0(8)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{PF}_6)(\text{tpa})(\text{MeCN})]_n$.

	x	y	z	U(eq)
H(2)	-1689	3988	123	62
H(3)	753	4309	-489	70
H(4)	4090	4515	-183	69
H(5)	4896	4365	671	67
H(7)	244	2899	588	72
H(8)	-1444	2059	391	94
H(9)	-4768	1911	709	95
H(10)	-6222	2566	1246	80
H(11)	-1325	3439	2095	47
H(13)	-1629	4857	1235	56
H(14)	-1939	5369	2009	62
H(15)	-1858	4905	2799	56
H(17A)	2801	1608	2636	239
H(17B)	530	1761	2807	239
H(17C)	2424	2015	3115	239

Table 1. Crystal data and structure refinement for $[\text{Ag}(\text{ClO}_4)(\text{tpa})(\text{MeCN})]_n$.

Identification code	5	
Empirical formula	C17 H15 Ag Cl N5 O4	
Formula weight	496.66	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 6.4275(12) Å	$\alpha = 90^\circ$.
	b = 23.160(5) Å	$\beta = 90^\circ$.
	c = 24.887(5) Å	$\gamma = 90^\circ$.
Volume	3704.8(13) Å ³	
Z	8	
Density (calculated)	1.781 Mg/m ³	
Absorption coefficient	1.268 mm ⁻¹	
F(000)	1984	
Crystal size	.1 x .1 x .4 mm ³	
Theta range for data collection	1.64 to 28.46°.	
Index ranges	-8 ≤ h ≤ 8, -29 ≤ k ≤ 27, -28 ≤ l ≤ 32	
Reflections collected	25112	
Independent reflections	4528 [R(int) = 0.1354]	
Completeness to theta = 28.46°	96.5 %	
Absorption correction	Empirical	
Max. and min. transmission	0.2753 and 0.2277	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4528 / 0 / 289	
Goodness-of-fit on F ²	0.794	
Final R indices [I > 2σ(I)]	R1 = 0.0525, wR2 = 0.1013	
R indices (all data)	R1 = 0.2281, wR2 = 0.1382	
Largest diff. peak and hole	0.690 and -0.848 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² × 10³) for $[\text{Ag}(\text{ClO}_4)(\text{tpa})(\text{MeCN})]_n$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	3674(1)	3740(1)	1664(1)	80(1)
Cl(1)	1464(6)	987(1)	1292(1)	77(1)
O(1)	2030(50)	509(13)	1101(12)	172(15)
O(1A)	1170(60)	367(15)	1175(12)	190(20)
O(2)	1810(30)	1324(13)	803(7)	98(8)
O(2A)	1700(50)	1424(14)	1009(16)	240(20)
O(3)	-850(30)	994(10)	1321(8)	106(7)
O(3A)	50(50)	1127(14)	1626(19)	230(20)
O(4)	2000(60)	1130(20)	1765(14)	270(20)
O(4A)	3410(30)	1016(9)	1561(9)	154(10)
N(1)	2137(9)	4091(3)	874(2)	52(2)
N(2)	-4041(10)	3136(3)	1216(2)	54(2)
N(3)	-1655(8)	4151(3)	2535(2)	44(2)
N(4)	-1213(9)	3768(3)	1099(2)	47(1)
N(5)	1859(19)	2722(5)	2120(5)	140(4)
C(1)	189(11)	3989(3)	709(3)	40(2)
C(2)	-407(12)	4077(3)	188(3)	52(2)
C(3)	1039(14)	4263(4)	-182(3)	67(2)
C(4)	2979(14)	4380(4)	-19(4)	68(3)
C(5)	3481(13)	4296(4)	511(3)	68(3)
C(6)	-2148(11)	3230(4)	1014(3)	41(2)

C(7)	-1102(13)	2809(4)	709(3)	62(2)
C(8)	-2017(18)	2304(4)	615(4)	86(3)
C(9)	-3960(20)	2204(4)	817(4)	100(4)
C(10)	-4898(14)	2616(5)	1108(4)	73(3)
C(11)	-1479(10)	3851(3)	2069(3)	47(2)
C(12)	-1496(10)	4104(3)	1570(3)	39(2)
C(13)	-1717(11)	4692(4)	1554(3)	53(2)
C(14)	-1843(12)	5011(3)	2022(4)	58(2)
C(15)	-1829(11)	4723(5)	2498(3)	53(2)
C(16)	1700(40)	2329(8)	2376(7)	202(9)
C(17)	1720(40)	1830(7)	2765(6)	310(13)

Table 3. Bond lengths [Å] and angles [°] for $[\text{Ag}(\text{ClO}_4)(\text{tpa})(\text{MeCN})]_n$.

Ag(1)-N(3)#1	2.216(6)
Ag(1)-N(2)#2	2.316(6)
Ag(1)-N(1)	2.346(6)
Cl(1)-O(2A)	1.24(3)
Cl(1)-O(1)	1.26(2)
Cl(1)-O(3A)	1.27(3)
Cl(1)-O(4)	1.27(3)
Cl(1)-O(4A)	1.423(18)
Cl(1)-O(2)	1.46(2)
Cl(1)-O(1A)	1.48(3)
Cl(1)-O(3)	1.486(17)
N(1)-C(5)	1.337(9)
N(1)-C(1)	1.340(8)
N(2)-C(6)	1.335(8)
N(2)-C(10)	1.350(10)
N(3)-C(15)	1.334(9)
N(3)-C(11)	1.357(8)
N(4)-C(6)	1.399(9)
N(4)-C(12)	1.419(8)
N(4)-C(1)	1.421(8)
N(5)-C(16)	1.116(16)
C(1)-C(2)	1.367(9)
C(2)-C(3)	1.377(9)
C(3)-C(4)	1.339(10)
C(4)-C(5)	1.372(10)
C(6)-C(7)	1.406(10)
C(7)-C(8)	1.330(11)
C(8)-C(9)	1.367(13)
C(9)-C(10)	1.342(12)
C(11)-C(12)	1.375(8)
C(12)-C(13)	1.370(9)
C(13)-C(14)	1.383(10)
C(14)-C(15)	1.359(10)
C(16)-C(17)	1.507(18)
N(3)#1-Ag(1)-N(2)#2	138.8(2)
N(3)#1-Ag(1)-N(1)	124.4(2)
N(2)#2-Ag(1)-N(1)	94.2(2)
O(2A)-Cl(1)-O(1)	118(2)
O(2A)-Cl(1)-O(3A)	104(3)
O(1)-Cl(1)-O(3A)	133(2)
O(2A)-Cl(1)-O(4)	106(3)
O(1)-Cl(1)-O(4)	120(3)

O(2A)-Cl(1)-O(4A)	97(2)
O(1)-Cl(1)-O(4A)	88.0(17)
O(3A)-Cl(1)-O(4A)	108(2)
O(1)-Cl(1)-O(2)	96.5(18)
O(3A)-Cl(1)-O(2)	121(2)
O(4)-Cl(1)-O(2)	126(2)
O(4A)-Cl(1)-O(2)	103.5(13)
O(3A)-Cl(1)-O(1A)	106.7(19)
O(4)-Cl(1)-O(1A)	118(2)
O(4A)-Cl(1)-O(1A)	104.5(15)
O(2)-Cl(1)-O(1A)	112.0(16)
O(2A)-Cl(1)-O(3)	98.0(18)
O(1)-Cl(1)-O(3)	108.5(16)
O(4)-Cl(1)-O(3)	102.9(19)
O(2)-Cl(1)-O(3)	100.7(11)
O(1A)-Cl(1)-O(3)	84.0(15)
C(5)-N(1)-C(1)	117.3(7)
C(5)-N(1)-Ag(1)	114.7(5)
C(1)-N(1)-Ag(1)	126.2(5)
C(6)-N(2)-C(10)	116.3(7)
C(6)-N(2)-Ag(1)#3	131.3(6)
C(10)-N(2)-Ag(1)#3	112.1(6)
C(15)-N(3)-C(11)	117.1(7)
C(15)-N(3)-Ag(1)#4	119.8(6)
C(11)-N(3)-Ag(1)#4	122.7(6)
C(6)-N(4)-C(12)	123.9(6)
C(6)-N(4)-C(1)	119.3(6)
C(12)-N(4)-C(1)	116.7(6)
N(1)-C(1)-C(2)	121.8(7)
N(1)-C(1)-N(4)	116.5(6)
C(2)-C(1)-N(4)	121.6(6)
C(1)-C(2)-C(3)	119.4(7)
C(4)-C(3)-C(2)	119.3(8)
C(3)-C(4)-C(5)	118.8(8)
N(1)-C(5)-C(4)	123.2(8)
N(2)-C(6)-N(4)	118.8(7)
N(2)-C(6)-C(7)	121.7(8)
N(4)-C(6)-C(7)	119.6(7)
C(8)-C(7)-C(6)	119.6(9)
C(7)-C(8)-C(9)	119.3(10)
C(10)-C(9)-C(8)	119.2(10)
C(9)-C(10)-N(2)	124.0(9)
N(3)-C(11)-C(12)	123.7(7)
C(13)-C(12)-C(11)	116.8(7)
C(13)-C(12)-N(4)	122.3(6)
C(11)-C(12)-N(4)	120.8(7)
C(12)-C(13)-C(14)	120.9(7)
C(15)-C(14)-C(13)	118.1(8)
N(3)-C(15)-C(14)	123.4(8)
N(5)-C(16)-C(17)	173(2)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, y, -z+1/2$ #2 $x+1, y, z$ #3 $x-1, y, z$ #4 $x-1/2, y, -z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ag}(\text{ClO}_4)(\text{tpa})(\text{MeCN})]_n$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
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Ag(1)	60(1)	134(1)	44(1)	-10(1)	3(1)	-7(1)
Cl(1)	91(2)	73(2)	67(2)	-3(2)	10(2)	-1(2)
O(1)	230(30)	66(19)	220(30)	-62(18)	100(20)	27(18)
O(1A)	300(40)	110(20)	170(20)	49(17)	-120(30)	-130(30)
O(2)	68(11)	180(20)	47(8)	18(11)	20(6)	24(13)
O(2A)	210(30)	190(30)	340(50)	220(40)	60(30)	-30(20)
O(3)	52(11)	125(17)	142(16)	37(13)	26(10)	-5(11)
O(3A)	140(30)	240(30)	320(50)	-150(30)	80(30)	-90(20)
O(4)	230(40)	440(50)	150(20)	-190(30)	0(20)	-90(40)
O(4A)	153(19)	144(18)	160(20)	14(16)	-131(19)	24(16)
N(1)	45(4)	70(5)	42(4)	-3(4)	4(3)	6(4)
N(2)	50(5)	59(5)	52(4)	-2(4)	-10(3)	-16(4)
N(3)	23(4)	73(5)	37(4)	0(4)	-3(3)	-2(4)
N(4)	48(3)	52(4)	39(3)	-9(3)	11(3)	-3(4)
N(5)	155(10)	88(9)	176(12)	19(8)	12(9)	-13(7)
C(1)	34(4)	48(6)	38(5)	-5(4)	2(4)	1(4)
C(2)	49(5)	69(6)	37(5)	-11(4)	-8(4)	-15(4)
C(3)	69(7)	90(7)	42(5)	-4(4)	9(5)	-12(6)
C(4)	74(7)	74(7)	56(6)	11(5)	27(5)	-12(5)
C(5)	52(5)	90(7)	60(6)	5(5)	16(5)	-12(6)
C(6)	39(5)	46(6)	37(5)	1(4)	-4(4)	-18(4)
C(7)	59(6)	51(7)	77(6)	-1(5)	13(5)	-5(5)
C(8)	119(10)	44(7)	96(8)	-20(6)	22(7)	-23(7)
C(9)	143(12)	42(7)	113(10)	3(7)	-18(9)	-27(8)
C(10)	67(6)	75(9)	75(7)	2(6)	6(5)	-22(6)
C(11)	36(4)	59(6)	44(4)	3(4)	-3(4)	-1(5)
C(12)	31(4)	39(5)	45(5)	8(4)	4(4)	11(4)
C(13)	53(5)	64(7)	42(5)	1(4)	9(4)	11(5)
C(14)	56(6)	36(6)	83(7)	0(5)	4(5)	-5(4)
C(15)	35(5)	62(8)	63(6)	-18(5)	6(4)	6(5)
C(16)	360(20)	103(15)	148(16)	-13(11)	124(16)	-17(18)
C(17)	630(40)	106(14)	189(18)	33(12)	80(30)	70(20)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $[\text{Ag}(\text{ClO}_4)(\text{tpa})(\text{MeCN})]_n$.

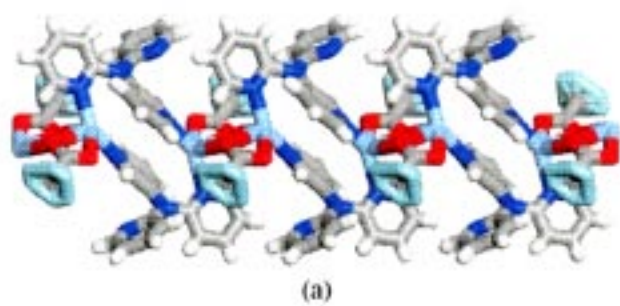
	x	y	z	U(eq)
H(2)	-1777	4011	84	62
H(3)	672	4307	-541	80
H(4)	3969	4515	-261	82
H(5)	4822	4386	624	81
H(7)	222	2883	575	75
H(8)	-1341	2022	414	103
H(9)	-4630	1854	752	120
H(10)	-6218	2540	1244	87
H(11)	-1338	3452	2089	56
H(13)	-1783	4879	1223	64
H(14)	-1933	5412	2012	70
H(15)	-1948	4936	2813	64
H(17A)	2985	1615	2723	465
H(17B)	551	1583	2693	465
H(17C)	1628	1974	3126	465

Supplementary materials - figures

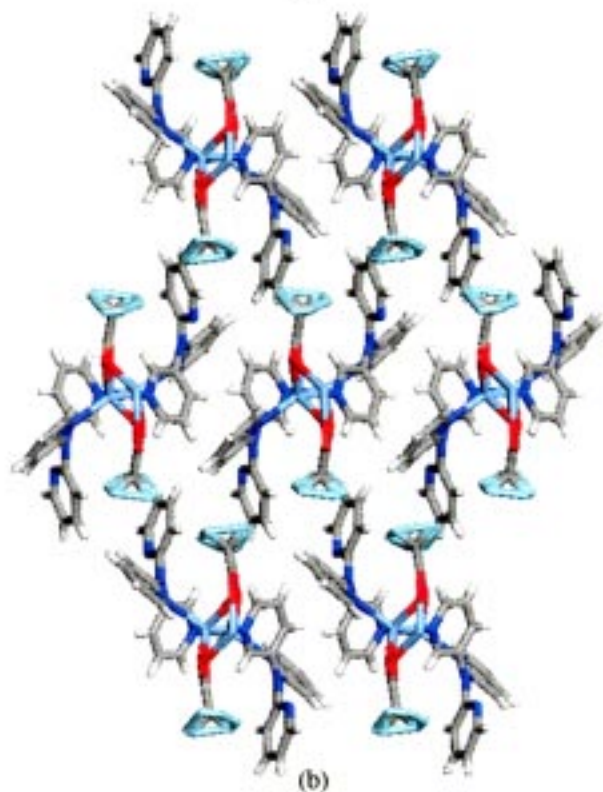
Anion Dependent Structures of Luminescent Silver(I) complexes

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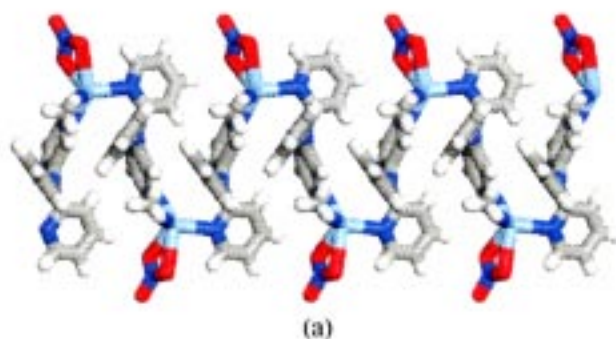


(a)

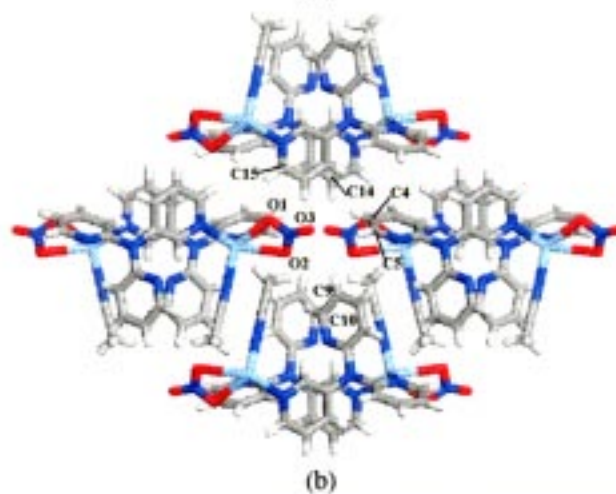


(b)

Figure S1. (a) Top view of one chain of **1**, showing the linked dimer units. (b) View down the chain axis, showing inter-chain packing.



(a)



(b)

Figure S2. (a) Top view of one chain of **2**, showing the zigzag coordination polymer. (b) View down the chain axis, showing inter-chain packing. Carbon and oxygen atoms involved in H-bonding interactions are labelled.

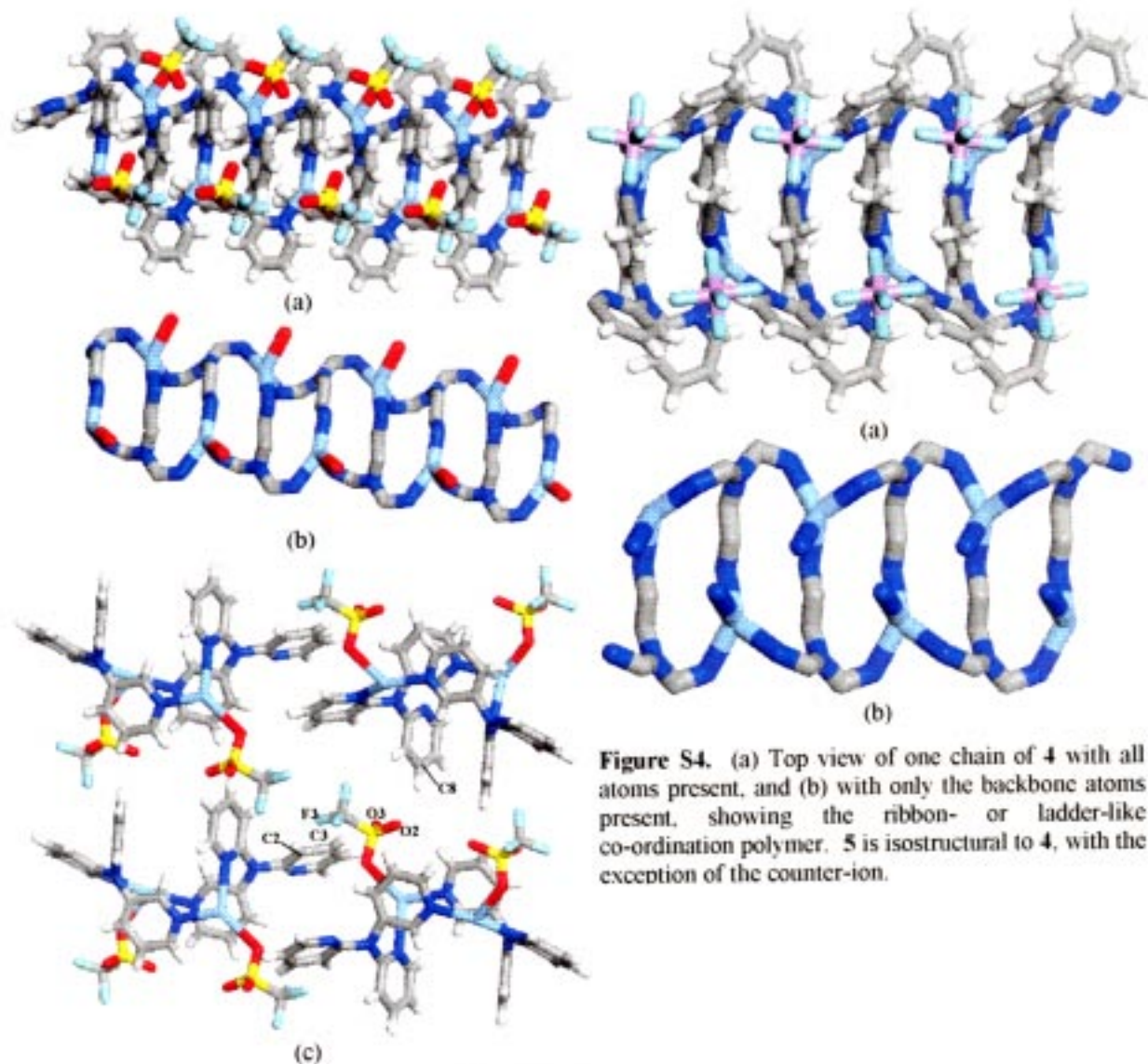


Figure S4. (a) Top view of one chain of **4** with all atoms present, and (b) with only the backbone atoms present, showing the ribbon- or ladder-like co-ordination polymer. **5** is isostructural to **4**, with the exception of the counter-ion.

Figure S3. (a) Top view of one chain of **3** with all atoms present, and (b) with only the backbone atoms present, showing the ribbon- or ladder-like co-ordination polymer. (c) View down the chain axis, showing inter-chain packing. Carbon, oxygen and fluorine atoms involved in hydrogen bonding are labelled.

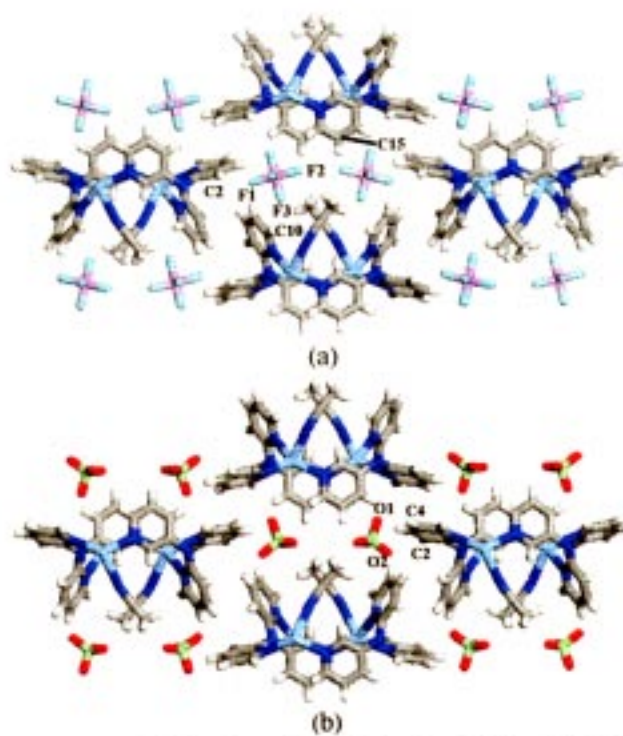


Figure S5. View down the chain axis of (a) 4 and (b) 5, showing inter-chain packing. Carbon, oxygen, and fluorine atoms involved in H-bonding interactions are labelled.