

Supporting Information

Synthesis and Characterization of Novel Simultaneous C and O- Coordinated and Nitrate-Bridged Complexes of Silver(I) with Carbonyl-Stabilized Sulfonium Ylides and Their Antibacterial Activities

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2.5.1. Synthesis of ylides $(Me)_2SCHC(O)C_6H_4R$ ($R = H; p-NO_2; p-OCH_3; p-Me$ and $p-Br$)

(Me)₂SCHC(O)C₆H₅: To an acetone solution (10 ml) of dimethylsulfide (0.062 g, 1.00 mmol) was added 2-bromoacetophenone (0.199 g, 1.00 mmol) and the mixture was stirred for 12 h. The solid product (sulfonium salt) was isolated by filtration, washed with ether and dried under reduced pressure. Further treatment with aqueous 10% NaOH solution led to elimination of HBr, giving the free ligand.²⁸ IR (KBr disk): ν (cm⁻¹) 1580 (C=O) and 865 (S–C). ¹H NMR (CDCl₃): δ (ppm) 2.85 (s, 6H, S(CH₃)₂); 4.23 (1H, CH); 7.41 (m, 3H, Ph); 7.80 (d, $^3J_{HH} = 8.1$ Hz, 2H, Ph). ¹³C-NMR (CDCl₃, ppm): δ 28.75 (s, S(CH₃)₂); 53.64 (s, CH); 126.30 (s, Ph(*p*)); 127.84 (s, Ph(*m*)); 129.42 (s, Ph(*o*)); 140.87 (s, Ph(*i*)); 182.50 (s, CO).

(Me)₂SCHC(O)C₆H₄-*p*-NO₂: Ylide was prepared following the same synthetic method as that reported for ligand **(Me)₂SCHC(O)C₆H₅**. Thus, dimethylsulfide (0.062 g, 1.00 mmol) was reacted with 2-bromo-4'-nitroacetophenone (0.244 g, 1.00 mmol) giving the free ligand.²⁷ IR (KBr disk): ν (cm⁻¹) 1551 (C=O) and 875 (S–C). ¹H NMR (CDCl₃): δ (ppm) 2.92 (s, 6H, S(CH₃)₂); 4.21 (1H, CH); 7.78 (d, $^3J_{HH} = 8.1$ Hz, 2H, Ph); 8.1 (d, $^3J_{HH} = 8.5$ Hz, 2H, Ph). ¹³C-NMR (CDCl₃, ppm): δ 28.26 (s, S(CH₃)₂); 54.26 (s, CH); 123.09 (s, Ph(*m*)); 127.23 (s, Ph(*o*)); 128.4 (s, Ph(*i*)); 146.84 (s, Ph(*p*)); 180.09 (s, CO).

(Me)₂SCHC(O)C₆H₄-*p*-OCH₃: Ylide was prepared following the same synthetic method as that reported for ligand **(Me)₂SCHC(O)C₆H₅**. Thus, dimethylsulfide (0.062 g, 1.00 mmol) was reacted with 2-bromo-4'-methoxyacetophenone (0.211 g, 1.00 mmol) giving the free ligand.²⁸ IR (KBr disk): ν (cm⁻¹) 1583 (C=O) and 857 (S–C). ¹H NMR (CDCl₃): δ (ppm) 2.96 (s, 6H, S(CH₃)₂); 3.79 (s, 3H, OCH₃); 4.27 (1H, CH); 6.83 (d, $^3J_{HH} = 8.0$ Hz, 2H, Ph); 7.74 (d, $^3J_{HH} = 8.0$ Hz, 2H, Ph). ¹³C-NMR (CDCl₃, ppm): δ 28.71 (s, S(CH₃)₂); 50.54 (s, OCH₃); 55.23 (s, CH); 113.10 (s, Ph(*p*)); 127.95 (s, Ph(*m*)); 133.45 (s, Ph(*o*)); 160.90 (s, Ph(*i*)); 182.77 (s, CO).

(Me)₂SCHC(O)C₆H₄-p-Me: Ylide was prepared following the same synthetic method as that reported for ligand **(Me)₂SCHC(O)C₆H₅:** Thus, dimethylsulfide (0.062 g, 1.00 mmol) was reacted with 2-bromo-4'-methylacetophenone (0.213 g, 1.00 mmol) giving the free ligand.²⁶ IR (KBr disk): ν (cm⁻¹) 1564 (C=O) and 879 (S–C). ¹H NMR (CDCl₃): δ (ppm) 2.32 (s, 3H, CH₃); 2.93 (s, 6H, S(CH₃)₂); 4.28 (1H, CH); 7.10 (d, ³J_{HH} = 8.1 Hz, 2H, arom.); 7.65 (d, ³J_{HH} = 8.1 Hz, 2H, arom.). ¹³C-NMR (CDCl₃, ppm): δ 20.80 (s, CH₃); 28.33 (s, S(CH₃)₂); 50.33 (s, CH); 125.98 (s, Ph(*p*)); 128.13 (s, Ph(*m*)); 138.08 (s, Ph(*o*)); 138.96 (s, Ph(*i*)); 182.32 (s, CO).

(Me)₂SCHC(O)C₆H₄-p-Br: Ylide was prepared following the same synthetic method as that reported for ligand **(Me)₂SCHC(O)C₆H₅:** Thus, dimethylsulfide (0.062 g, 1.00 mmol) was reacted with 2-bromo-4'-bromoacetophenone (0.260 g, 1.00 mmol) giving the free ligand.²⁷ IR (KBr disk): ν (cm⁻¹) 1578 (C=O) and 855 (S–C). ¹H NMR (CDCl₃): δ (ppm) 2.91 (s, 6H, S(CH₃)₂); 4.24 (1H, CH); 7.42 (d, ³J_{HH} = 8.1 Hz, 2H, Ph); 7.60 (d, ³J_{HH} = 8.1 Hz, 2H, Ph). ¹³C-NMR (CDCl₃, ppm): δ 28.15 (s, S(CH₃)₂); 52.27 (s, CH); 123.00 (s, Ph(*m*)); 127.64 (s, Ph(*p*)); 130.39 (s, Ph(*i*)); 139.66 (s, Ph(*o*)); 180.49 (s, CO).

[AgNO₃(Me₂SCHC(O)C₆H₅)]_n (1)

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-assg. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	x	y	z	U(eq)
Ag1	5089.7(2)	6340.1(2)	5568.78(7)	26.82(9)
S1	1465.3(8)	6774.3(7)	5870.3(2)	22.83(14)
O1	3195(3)	8263(2)	6514.8(7)	28.7(4)
C1	3280(3)	6136(3)	6080.9(8)	19.4(5)
C2	3771(3)	7050(3)	6444.2(8)	20.4(5)
C3	4993(3)	6445(3)	6750.6(9)	20.5(5)
C4	5897(4)	5230(3)	6646.1(10)	28.4(6)
C5	6947(4)	4648(4)	6946.9(11)	37.1(7)
C6	7110(4)	5279(4)	7355.7(11)	35.0(7)
C7	6237(4)	6502(3)	7459.9(10)	30.9(6)
C8	5179(3)	7087(3)	7160.0(9)	24.6(6)
C9	21(3)	6409(3)	6290.8(11)	29.9(7)
C10	982(4)	5346(3)	5500.2(9)	29.9(6)
O2	5910(3)	3868(2)	5236.4(7)	30.9(4)
N1	7075(3)	3246(3)	5408.9(7)	22.6(5)
O3	7631(3)	3682(3)	5758.2(7)	37.2(5)
O4	7676(3)	2161(2)	5216.5(7)	33.2(5)

Table S2. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-assg. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka \times b \times U_{12}]$

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ag1	26.83(13)	28.09(14)	25.54(13)	-0.44(7)	5.36(7)	-1.95(7)
S1	23.5(3)	21.1(3)	23.9(3)	1.2(2)	-5.4(2)	1.3(2)
O1	34.8(11)	20.6(9)	30.7(10)	-4.3(8)	-6.9(9)	6.6(8)
C1	18.1(12)	17.5(12)	22.6(12)	2.4(9)	-1.0(9)	0.0(9)
C2	19.5(12)	19.3(12)	22.4(12)	1.9(9)	1.7(10)	-1.9(10)
C3	19.6(12)	21.8(14)	20.0(13)	1.8(10)	-0.6(9)	-4.2(9)
C4	27.1(14)	27.2(14)	30.9(14)	-1.6(11)	-4.5(11)	2.9(11)
C5	34.4(16)	29.7(16)	47.3(18)	0.8(13)	-14.2(14)	6.2(13)
C6	31.6(15)	33.5(16)	39.9(16)	13.4(13)	-14.2(13)	-7.5(13)
C7	31.0(15)	37.8(16)	23.8(13)	4.8(12)	-5.1(11)	-13.8(13)
C8	22.6(13)	26.5(15)	24.6(13)	-0.5(11)	1.6(10)	-5(1)
C9	23.9(14)	36.2(17)	29.5(15)	-0.4(12)	0.2(10)	4.4(11)
C10	31.5(15)	29.8(15)	28.5(14)	-4.5(11)	-7.1(11)	-3.8(12)
O2	29.4(10)	34.4(11)	29(1)	-0.3(8)	-4.6(8)	10.1(9)
N1	22.8(11)	23.4(11)	21.7(11)	2.9(9)	2.0(9)	-1.1(9)
O3	35.3(12)	46.9(13)	29.3(11)	-10.3(9)	-7.9(9)	2.2(10)
O4	35.3(11)	28.8(11)	35.6(11)	-8.3(9)	-7.7(9)	11.4(9)

Table S3. Bond Lengths for fa-assg.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	C1	2.198(3)	C3	C8	1.393(4)
Ag1	O2	2.590(2)	C4	C5	1.386(4)
Ag1	O4 ¹	2.303(2)	C5	C6	1.385(5)
S1	C1	1.765(3)	C6	C7	1.385(5)
S1	C9	1.805(3)	C7	C8	1.390(4)
S1	C10	1.784(3)	O2	N1	1.256(3)
O1	C2	1.239(3)	N1	O3	1.234(3)
C1	C2	1.454(4)	N1	O4	1.267(3)
C2	C3	1.502(4)	O4	Ag1 ²	2.302(2)
C3	C4	1.393(4)			

¹3/2-X,1/2+Y,+Z; ²3/2-X,-1/2+Y,+Z

Table S4. Bond Angles for fa-assg.

Atom	Atom	Atom	Angle/ [°]	Atom	Atom	Atom	Angle/ [°]
C1	Ag1	O2	113.00(8)	C4	C3	C8	119.1(3)
C1	Ag1	O4 ¹	158.88(9)	C8	C3	C2	118.7(2)
O4 ¹	Ag1	O2	83.46(7)	C5	C4	C3	120.7(3)
C1	S1	C9	105.45(13)	C6	C5	C4	120.0(3)
C1	S1	C10	100.63(14)	C7	C6	C5	119.8(3)
C10	S1	C9	99.12(15)	C6	C7	C8	120.5(3)
S1	C1	Ag1	108.50(12)	C7	C8	C3	120.0(3)
C2	C1	Ag1	107.18(17)	N1	O2	Ag1	116.60(16)
C2	C1	S1	109.49(18)	O2	N1	O4	118.8(2)
O1	C2	C1	123.0(2)	O3	N1	O2	120.8(2)
O1	C2	C3	119.8(2)	O3	N1	O4	120.4(2)
C1	C2	C3	117.2(2)	N1	O4	Ag1 ²	111.84(16)
C4	C3	C2	122.2(3)				

¹3/2-X,1/2+Y,+Z; ²3/2-X,-1/2+Y,+Z

Table S5. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-assg.

Atom	x	y	z	U(eq)
H1	3179	5104	6177	23
H4	5793	4796	6366	34
H5	7554	3817	6873	45
H6	7819	4875	7564	42
H7	6362	6943	7739	37
H8	4583	7925	7234	29
H9A	192	5433	6408	45
H9B	-1044	6473	6166	45
H9C	132	7123	6526	45
H10A	1807	5268	5276	45
H10B	-35	5555	5360	45
H10C	908	4429	5661	45

[Ag(Me₂SCHC(O)C₆H₄-*m*-NO₂)₂]₂(NO₃)₂·2H₂O (2)

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-agmGau. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	x	y	z	U(eq)
Ag1	4751.3(3)	1852.7(3)	2011.78(15)	28.84(11)
S1	7380.7(12)	2357.1(12)	1273.0(5)	29.6(2)
S2	2005.9(12)	2120.6(12)	2819.7(5)	27.9(2)
O7	7465(4)	2899(3)	2391.2(15)	28.7(7)
O8	7444(4)	734(4)	4995.5(17)	45(1)
O9	7153(5)	2584(4)	4488.6(18)	45(1)
O10	1281(4)	3884(4)	1838.5(15)	32.3(8)
O11	1273(11)	5868(6)	-128(3)	109(3)
O12	1857(7)	4812(6)	-844(2)	73.7(17)
N1	7233(5)	1457(5)	4540.4(19)	36(1)
N2	1720(8)	4874(7)	-321(2)	60.7(17)
C1	6910(5)	1465(5)	1907(2)	26.1(9)
C2	7043(7)	1604(6)	716(3)	46.0(14)
C3	9159(6)	1843(7)	1219(3)	48.0(15)
C4	7052(5)	1129(4)	2995(2)	24.9(9)
C5	6731(5)	3(5)	3064(2)	29.6(10)
C6	6562(6)	-639(5)	3617(2)	35.3(11)
C7	6738(5)	-169(5)	4099(2)	33.5(11)
C8	7071(5)	936(5)	4023(2)	29.3(10)
C9	7231(5)	1612(5)	3486(2)	26.5(9)
C10	2678(5)	1820(5)	2113(2)	27.5(10)
C11	7181(4)	1896(4)	2416(2)	24.8(9)
C12	523(5)	1653(5)	2884(2)	33.8(11)
C13	2012(5)	2854(5)	1696(2)	28.7(10)
C14	2277(6)	2704(5)	1063(2)	33.5(11)
C15	3059(6)	842(6)	3271(2)	38.8(12)
C16	2926(9)	1551(7)	852(3)	57.5(18)
C17	3160(11)	1495(9)	266(4)	75(3)
C18	2743(10)	2577(9)	-131(3)	67(2)
C19	2112(7)	3707(7)	84(3)	46.8(15)
C20	1862(6)	3788(6)	670(2)	37.5(12)
Ag2	1028.3(3)	5557.4(4)	2768.25(15)	30.75(12)
S3	3589.0(11)	5035.5(12)	1804.9(5)	28.2(2)
S4	-1679.1(11)	4884.9(11)	2926.6(5)	25.0(2)
O1	-1188(4)	4895(4)	4085.7(15)	32.1(8)

O2	-1379(4)	7103(4)	5772.2(17)	40.7(9)
O3	-243(5)	8418(4)	5707.9(18)	44.2(10)
O4	4308(4)	3344(4)	2861.8(17)	34.7(8)
O5	4432(5)	1871(4)	4890(2)	47.1(11)
O6	4041(5)	3164(4)	5528.8(17)	45.5(10)
N6	5518(9)	8540(12)	1791(4)	54.9(15)
O18	5758(10)	8379(11)	2293(4)	61.9(8)
O17	4413(9)	8610(11)	1659(4)	61.9(8)
O16	6336(9)	8675(11)	1395(4)	61.9(8)
N7	3788(11)	8482(12)	2332(5)	54.9(15)
O19	4937(10)	8226(11)	2480(5)	61.9(8)
O21	2641(11)	8528(12)	2629(5)	61.9(8)
O20	3827(12)	8674(11)	1785(4)	61.9(8)
N8	1312(19)	8920(20)	2250(8)	54.9(15)
O23	1630(20)	9380(20)	1763(8)	61.9(8)
O22	2040(20)	8610(20)	2657(9)	61.9(8)
O24	206(18)	8860(20)	2307(9)	61.9(8)
N9	-270(20)	8580(20)	1772(8)	54.9(15)
O27	-870(20)	8420(20)	1392(8)	61.9(8)
O26	702(19)	8990(20)	1777(9)	61.9(8)
O25	-750(20)	8280(20)	2248(8)	61.9(8)
N3	4118(5)	2945(5)	5028(2)	35.8(10)
N4	-700(4)	7722(5)	5498.7(19)	33.6(10)
C21	3087(5)	5454(5)	2508(2)	28.5(10)
C22	5122(5)	5402(6)	1637(2)	34.3(11)
C23	2502(6)	6308(6)	1366(2)	40.9(13)
C24	3725(5)	4461(5)	2949(2)	28.8(10)
C25	3622(5)	4775(5)	3560(2)	25.8(9)
C26	3927(5)	3769(5)	3998(2)	27.9(10)
C27	3827(5)	4020(5)	4564(2)	28.5(10)
C28	3441(5)	5228(5)	4713(2)	29.8(10)
C29	3181(5)	6236(5)	4265(2)	31.5(10)
C30	3257(5)	6017(5)	3696(2)	28.4(10)
C31	-1009(5)	5988(5)	3141(2)	25.9(9)
C32	-3402(5)	5346(6)	3168(2)	33.4(11)
C33	-1764(5)	5420(5)	2164(2)	28.7(10)
C34	-951(5)	5794(5)	3771(2)	26.2(9)
C35	-585(5)	6778(5)	4030(2)	25.3(9)
C36	-763(5)	6753(5)	4632(2)	25.2(9)
C37	-116(5)	7717(5)	3693(2)	28.1(10)
C38	228(5)	8600(5)	3949(2)	32.4(11)
C39	-440(5)	7673(5)	4870(2)	27.4(10)
C40	69(5)	8580(5)	4543(2)	32.2(11)

O13	4964(12)	4217(12)	-260(5)	61.9(8)
O14	4682(11)	4162(11)	619(5)	61.9(8)
O15	4541(12)	5921(12)	181(5)	61.9(8)
N5	4809(10)	4727(12)	130(5)	54.9(15)
O28	3879.3(18)	8335(7)	556(2)	77.2(17)
O29	974(12)	9192(12)	405(6)	77.2(17)
O30	18(15)	1454(16)	9689(7)	77.2(17)
O31	1677(4)	9380(20)	575.0(18)	77.2(17)

Table S2. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-agmGau. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*{}^2U_{11} + \dots + 2hka \times b \times U_{12}]$

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ag1	22.41(18)	35.0(2)	31.07(19)	-10.27(14)	0.88(13)	-9.42(14)
S1	29.2(6)	33.1(6)	24.9(5)	-5.9(4)	0.7(4)	-6.8(5)
S2	23.5(5)	34.6(6)	24.2(5)	-4.0(4)	-1.4(4)	-6.9(4)
O7	34.9(19)	27.8(17)	27.2(16)	-2.6(13)	-1.6(14)	-15.7(14)
O8	45(2)	55(3)	27.8(19)	0.1(17)	-3.5(17)	-7(2)
O9	59(3)	41(2)	36(2)	-13.1(17)	-3.1(19)	-12(2)
O10	27.1(18)	39(2)	29.0(17)	-4.7(14)	-1.5(14)	-7.2(15)
O11	205(8)	58(4)	47(3)	7(3)	-25(4)	-19(4)
O12	113(5)	94(4)	25(2)	4(2)	-9(3)	-52(4)
N1	31(2)	44(3)	28(2)	-7.3(19)	0.8(17)	-3.7(19)
N2	91(5)	69(4)	29(3)	4(3)	-11(3)	-36(4)
C1	25(2)	28(2)	26(2)	-7.7(18)	2.7(17)	-7.7(18)
C2	59(4)	51(4)	30(3)	-15(2)	-6(3)	-13(3)
C3	29(3)	65(4)	40(3)	6(3)	7(2)	-9(3)
C4	21(2)	22(2)	29(2)	-3.9(17)	-0.4(17)	-4.3(17)
C5	28(2)	23(2)	37(3)	-4.3(19)	-1.1(19)	-7.0(19)
C6	34(3)	30(3)	39(3)	1(2)	-2(2)	-10(2)
C7	29(3)	33(3)	32(3)	4(2)	2(2)	-6(2)
C8	26(2)	31(2)	26(2)	-3.7(19)	-0.4(18)	-2.5(19)
C9	25(2)	26(2)	27(2)	-5.7(18)	1.8(18)	-6.1(18)
C10	25(2)	34(2)	26(2)	-5.9(19)	2.4(18)	-13.3(19)
C11	19(2)	25(2)	29(2)	-4.9(17)	0.4(17)	-3.9(17)
C12	25(2)	42(3)	33(3)	0(2)	0.5(19)	-12(2)
C13	21(2)	40(3)	28(2)	-5(2)	-0.4(18)	-14(2)
C14	36(3)	41(3)	27(2)	-3(2)	0(2)	-18(2)
C15	30(3)	48(3)	30(3)	0(2)	-5(2)	-1(2)
C16	82(5)	46(4)	39(3)	-7(3)	-4(3)	-11(4)
C17	108(8)	62(5)	47(4)	-17(4)	4(4)	-11(5)
C18	105(7)	78(5)	26(3)	-8(3)	-2(3)	-38(5)
C19	62(4)	57(4)	29(3)	-2(3)	-5(3)	-30(3)
C20	45(3)	42(3)	29(3)	-4(2)	-5(2)	-19(3)
Ag2	19.08(18)	46.8(2)	28.85(19)	-12.71(15)	1.27(13)	-10.58(15)
S3	23.1(5)	37.7(6)	26.3(5)	-12.8(5)	1.9(4)	-9.8(5)
S4	21.2(5)	30.4(5)	25.1(5)	-6.7(4)	-1.1(4)	-8.5(4)
O1	38(2)	35.0(19)	27.3(17)	-5.6(14)	1.0(14)	-17.3(16)
O2	38(2)	58(3)	29.9(19)	-11.7(17)	7.0(16)	-19.5(19)
O3	53(3)	51(2)	37(2)	-21.4(18)	-2.4(18)	-21(2)
O4	26.4(18)	39(2)	38(2)	-18.5(16)	-2.4(15)	-2.1(15)
O5	53(3)	32(2)	51(2)	-3.2(18)	16(2)	-12.5(19)
O6	51(3)	51(2)	30(2)	-0.4(17)	2.9(17)	-14(2)

N3	32(2)	37(2)	36(2)	-0.0(19)	6.7(18)	-11.7(19)
N4	30(2)	43(2)	30(2)	-15.0(18)	-0.3(17)	-7.9(19)
C21	20(2)	42(3)	27(2)	-15(2)	2.5(17)	-10(2)
C22	27(3)	44(3)	35(3)	-11(2)	4(2)	-13(2)
C23	36(3)	54(3)	31(3)	-9(2)	-5(2)	-7(3)
C24	19(2)	41(3)	30(2)	-17(2)	1.8(17)	-9(2)
C25	19(2)	33(2)	29(2)	-13.0(19)	2.2(17)	-9.1(18)
C26	20(2)	34(2)	32(2)	-12.7(19)	6.3(18)	-10.6(19)
C27	23(2)	33(2)	30(2)	-5.5(19)	2.3(18)	-10.1(19)
C28	26(2)	39(3)	24(2)	-10.6(19)	-1.1(18)	-6(2)
C29	32(3)	30(2)	31(3)	-12(2)	-4(2)	-2(2)
C30	26(2)	30(2)	28(2)	-6.5(18)	-2.9(18)	-3.9(19)
C31	19(2)	34(2)	27(2)	-9.9(18)	0.3(17)	-9.3(18)
C32	23(2)	47(3)	36(3)	-13(2)	4.5(19)	-18(2)
C33	30(2)	38(3)	23(2)	-6.3(19)	-1.4(18)	-15(2)
C34	21(2)	32(2)	26(2)	-7.0(18)	1.1(17)	-8.1(18)
C35	19(2)	28(2)	29(2)	-6.6(18)	-2.1(17)	-5.1(17)
C36	21(2)	28(2)	27(2)	-6.7(18)	-0.1(17)	-6.4(18)
C37	26(2)	29(2)	29(2)	-4.0(18)	-1.7(18)	-5.9(19)
C38	31(3)	29(2)	38(3)	-6(2)	2(2)	-11(2)
C39	24(2)	32(2)	26(2)	-10.0(18)	-0.5(17)	-5.2(19)
C40	27(2)	28(2)	43(3)	-14(2)	-1(2)	-7(2)

Table S3. Bond Lengths for fa-agmGau.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	C1	2.192(5)	O1	C34	1.224(6)
Ag1	C10	2.202(5)	O2	N4	1.216(6)
S1	C1	1.766(5)	O3	N4	1.225(6)
S1	C2	1.788(6)	O4	C24	1.249(6)
S1	C3	1.793(6)	O5	N3	1.230(6)
S2	C10	1.767(5)	O6	N3	1.226(6)
S2	C12	1.795(5)	N6	O18	1.207(8)
S2	C15	1.791(5)	N6	O17	1.225(8)
O7	C11	1.243(6)	N6	O16	1.220(8)
O8	N1	1.228(6)	N7	O19	1.241(12)
O9	N1	1.226(7)	N7	O21	1.323(12)
O10	C13	1.245(7)	N7	O20	1.265(13)
O11	N2	1.206(9)	N8	O23	1.232(16)
O12	N2	1.228(8)	N8	O22	1.236(16)
N1	C8	1.476(7)	N8	O24	1.189(16)
N2	C19	1.461(9)	N9	O27	1.217(16)
C1	C11	1.447(7)	N9	O26	1.259(16)
C4	C5	1.387(7)	N9	O25	1.218(16)
C4	C9	1.403(7)	N3	C27	1.468(7)
C4	C11	1.501(7)	N4	C39	1.473(6)
C5	C6	1.400(7)	C21	C24	1.445(8)
C6	C7	1.374(8)	C24	C25	1.514(6)
C7	C8	1.371(8)	C25	C26	1.380(7)
C8	C9	1.382(7)	C25	C30	1.401(7)
C10	C13	1.443(7)	C26	C27	1.384(7)
C13	C14	1.505(7)	C27	C28	1.377(7)
C14	C16	1.400(9)	C28	C29	1.394(8)
C14	C20	1.384(8)	C29	C30	1.384(7)
C16	C17	1.375(10)	C31	C34	1.464(6)
C17	C18	1.390(12)	C34	C35	1.507(7)
C18	C19	1.380(11)	C35	C36	1.400(7)
C19	C20	1.381(8)	C35	C37	1.396(7)
Ag2	C21	2.177(5)	C36	C39	1.394(7)
Ag2	C31	2.177(5)	C37	C38	1.393(7)
S3	C21	1.763(5)	C38	C40	1.380(8)
S3	C22	1.789(5)	C39	C40	1.383(8)
S3	C23	1.789(6)	O13	N5	1.125(18)
S4	C31	1.766(5)	O14	N5	1.231(16)
S4	C32	1.792(5)	O15	N5	1.300(18)
S4	C33	1.794(5)			

Table S4. Bond Angles for fa-agmGau.

Atom	Atom	Atom	Angle/ [°]	Atom	Atom	Atom	Angle/ [°]
C1	Ag1	C10	168.19(19)	O18	N6	O16	122.3(8)
C1	S1	C2	101.9(3)	O16	N6	O17	117.2(8)
C1	S1	C3	105.5(3)	O19	N7	O21	132.8(12)
C2	S1	C3	100.8(3)	O19	N7	O20	107.9(11)
C10	S2	C12	103.0(2)	O20	N7	O21	119.2(11)
C10	S2	C15	102.9(3)	O23	N8	O22	123.5(19)
C15	S2	C12	101.3(3)	O24	N8	O23	114.3(18)
O8	N1	C8	118.0(5)	O24	N8	O22	122.1(19)
O9	N1	O8	124.1(5)	O27	N9	O26	134(2)
O9	N1	C8	117.9(4)	O27	N9	O25	110.6(18)
O11	N2	O12	122.3(7)	O25	N9	O26	114.9(18)
O11	N2	C19	118.5(6)	O5	N3	C27	117.8(5)
O12	N2	C19	119.2(7)	O6	N3	O5	123.8(5)
S1	C1	Ag1	111.0(2)	O6	N3	C27	118.4(5)
C11	C1	Ag1	102.2(3)	O2	N4	O3	124.3(5)
C11	C1	S1	110.3(3)	O2	N4	C39	118.5(4)
C5	C4	C9	119.5(5)	O3	N4	C39	117.2(5)
C5	C4	C11	123.3(4)	S3	C21	Ag2	113.2(2)
C9	C4	C11	117.2(4)	C24	C21	Ag2	99.2(3)
C4	C5	C6	120.6(5)	C24	C21	S3	111.9(4)
C7	C6	C5	120.1(5)	O4	C24	C21	123.9(4)
C8	C7	C6	118.5(5)	O4	C24	C25	117.9(5)
C7	C8	N1	118.6(5)	C21	C24	C25	118.0(4)
C7	C8	C9	123.5(5)	C26	C25	C24	117.0(4)
C9	C8	N1	117.9(5)	C26	C25	C30	119.5(4)
C8	C9	C4	117.8(5)	C30	C25	C24	123.4(5)
S2	C10	Ag1	109.5(2)	C25	C26	C27	118.7(5)
C13	C10	Ag1	104.1(3)	C26	C27	N3	118.4(5)
C13	C10	S2	109.5(4)	C28	C27	N3	118.4(5)
O7	C11	C1	122.1(4)	C28	C27	C26	123.2(5)
O7	C11	C4	119.5(4)	C27	C28	C29	117.6(5)
C1	C11	C4	118.4(4)	C30	C29	C28	120.5(5)
O10	C13	C10	122.6(5)	C29	C30	C25	120.4(5)
O10	C13	C14	118.9(5)	S4	C31	Ag2	106.3(2)
C10	C13	C14	118.5(5)	C34	C31	Ag2	107.0(3)
C16	C14	C13	124.1(5)	C34	C31	S4	110.2(4)
C20	C14	C13	117.1(5)	O1	C34	C31	123.4(5)
C20	C14	C16	118.7(5)	O1	C34	C35	120.1(4)
C17	C16	C14	120.8(7)	C31	C34	C35	116.5(4)
C16	C17	C18	120.9(8)	C36	C35	C34	117.6(4)
C19	C18	C17	117.6(6)	C37	C35	C34	122.7(4)

C18	C19	N2	119.1(6)	C37	C35	C36	119.6(4)
C18	C19	C20	122.6(6)	C39	C36	C35	117.6(5)
C20	C19	N2	118.3(6)	C38	C37	C35	121.0(5)
C19	C20	C14	119.4(6)	C40	C38	C37	120.1(5)
C31	Ag2	C21	167.05(18)	C36	C39	N4	118.7(5)
C21	S3	C22	103.7(2)	C40	C39	N4	117.9(4)
C21	S3	C23	102.3(3)	C40	C39	C36	123.3(5)
C23	S3	C22	101.0(3)	C38	C40	C39	118.4(5)
C31	S4	C32	106.2(2)	O13	N5	O14	120.0(14)
C31	S4	C33	100.5(2)	O13	N5	O15	131.9(14)
C32	S4	C33	101.1(3)	O14	N5	O15	107.3(13)
O18	N6	O17	120.5(8)				

Table S5. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-agmGau.

Atom	x	y	z	U(eq)
H1	7358	557	1905	31
H2A	7425	703	800	69
H2B	7422	1901	350	69
H2C	6102	1803	699	69
H3A	9479	2121	1526	72
H3B	9477	2197	852	72
H3C	9474	934	1252	72
H5	6628	-329	2739	36
H6	6330	-1384	3659	42
H7	6633	-590	4469	40
H9	7450	2363	3452	32
H10	2613	1011	2032	33
H12A	-115	2247	2638	51
H12B	163	1637	3279	51
H12C	730	824	2770	51
H15A	3179	59	3124	58
H15B	2658	801	3659	58
H15C	3905	981	3272	58
H16	3202	815	1111	69
H17	3604	722	134	90
H18	2884	2541	-528	81
H20	1419	4563	800	45
H21	3252	6251	2544	34
H22A	5008	6242	1719	51
H22B	5388	5354	1233	51
H22C	5792	4805	1867	51
H23A	1602	6310	1468	61
H23B	2723	6200	965	61
H23C	2600	7099	1430	61
H26	4193	2939	3915	34
H28	3357	5366	5098	36
H29	2956	7063	4350	38
H30	3063	6697	3402	34
H31	-1521	6859	3004	31
H32A	-3491	5212	3583	50
H32B	-3841	4847	3016	50
H32C	-3798	6227	3033	50
H33A	-2290	6293	2105	43
H33B	-2161	4918	1991	43
H33C	-885	5337	1988	43

H36	-1085	6144	4866	30
H37	-32	7753	3291	34
H38	565	9203	3720	39
H40	298	9163	4719	39
H28A	4691	8274	512	116
H28B	3477	8804	275	116
H29A	510(130)	9960(40)	360(90)	116
H29B	490(130)	8720(110)	420(110)	116
H30A	20(120)	1700(200)	9328(14)	116
H30B	650(160)	1600(200)	9820(70)	116
H31A	1303	9438	909	116
H31B	2491	9281	580	116

[Ag(Me₂SCHC(O)C₆H₄-*p*-NO₂)₂]₂[{AgNO₃(μ-NO₃)(Me₂SCHC(O)C₆H₄-*p*-NO₂)₂}₂. 2CH₃OH (3)]

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-asng. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Ag1	3111.78(18)	3903.35(18)	1415.91(16)	22.41(6)
Ag2	4765.3(2)	1749.73(19)	4536.84(18)	29.38(7)
S1	1260.1(6)	5843.2(6)	1292.0(5)	21.66(14)
S2	6072.7(6)	4073.7(6)	1028.7(5)	20.22(14)
S3	3128.9(6)	3815.6(6)	4915.2(5)	23.32(14)
O1	1368.6(17)	4577.7(17)	-61.2(14)	24.1(4)
O2	-2065(3)	-944(2)	2716.7(19)	49.1(7)
O3	-696(3)	-1103(2)	1369(2)	65.1(8)
O4	5737.0(17)	3816.0(17)	-675.9(14)	25.5(4)
O5	2410(3)	-1622(2)	617(2)	76.5(10)
O6	2666(3)	-652(2)	-868(2)	63.8(8)
O7	2582.5(18)	3358.2(16)	3416.7(15)	25.6(4)
O8	607(2)	-2630(2)	4687.3(19)	44.0(6)
O9	403(2)	-1649(2)	3301.7(19)	42.7(6)
O10	6902.4(19)	2349.6(18)	3835.9(16)	32.1(5)
O11	6156(2)	3853(2)	4159(2)	47.1(6)
O12	8136(2)	3787(2)	3566.7(19)	49.4(7)
O13	5057(2)	1147(2)	6372(2)	54.7(7)
O14	4393(3)	-209(2)	6068(2)	56.2(8)
O15	5153(3)	-602(3)	7197(2)	64.2(8)
N1	-1165(3)	-568(2)	1939(2)	39.2(7)
N2	2766(2)	-757(2)	-95(2)	32.0(6)
N3	708(2)	-1728(2)	4007(2)	31.8(6)
N4	7066(2)	3339(2)	3852.4(18)	30.2(6)
N5	4869(2)	103(2)	6570.2(19)	29.9(6)
C1	1211(2)	4343(2)	1588(2)	18.9(5)
C2	1068(2)	3973(2)	828(2)	18.2(5)
C3	511(2)	2752(2)	1166(2)	18.6(5)
C4	975(3)	2125(2)	522(2)	24.2(6)
C5	434(3)	1033(3)	777(2)	27.8(6)
C6	-584(3)	599(2)	1666(2)	25.4(6)
C7	-1082(3)	1202(2)	2309(2)	23.5(6)
C8	-509(2)	2281(2)	2059(2)	20.1(5)
C9	1518(3)	6010(3)	2323(2)	27.1(6)
C10	-327(3)	6127(3)	1596(2)	30.9(7)
C11	4897(2)	3161(2)	1103(2)	19.5(5)

C12	5097(2)	3085(2)	134(2)	19.0(5)
C13	4444(2)	2056(2)	120(2)	21.1(6)
C14	4456(3)	2080(3)	-796(2)	27.8(6)
C15	3907(3)	1157(3)	-875(2)	30.4(7)
C16	3362(3)	222(2)	-22(2)	25.6(6)
C17	3350(3)	152(3)	897(2)	30.3(7)
C18	3895(3)	1087(2)	958(2)	28.0(6)
C19	7097(3)	3085(3)	1403(2)	26.8(6)
C20	5414(3)	4453(3)	2130(2)	30.7(7)
C21	2917(3)	2426(2)	4896(2)	22.9(6)
C22	2543(2)	2453(2)	4097(2)	21.2(5)
C23	2093(2)	1327(2)	4096(2)	22.3(6)
C24	2138(3)	255(2)	4769(2)	27.2(6)
C25	1682(3)	-750(3)	4751(2)	28.0(6)
C26	1202(3)	-671(2)	4039(2)	25.8(6)
C27	1167(3)	368(3)	3350(2)	28.7(6)
C28	1597(3)	1364(2)	3394(2)	26.3(6)
C29	1595(3)	4229(3)	5399(3)	33.7(7)
C30	3533(3)	3517(3)	5982(2)	34.5(7)
O16	6660(2)	1962(2)	7060.4(18)	41.6(6)
C31	6588(3)	3095(3)	6511(3)	42.7(8)

C16	24.2(14)	17.9(14)	40.7(18)	-14.7(13)	-15.2(13)	5.2(11)
C17	40.3(17)	17.4(15)	34.9(17)	-3.9(13)	-20.1(15)	-2.8(12)
C18	38.8(16)	18.9(15)	29.7(16)	-7.0(12)	-17.9(14)	0.3(12)
C19	22.1(13)	25.7(16)	30.0(16)	-1.0(12)	-14.8(13)	3.0(11)
C20	35.1(16)	32.3(18)	35.4(17)	-16.6(14)	-20.5(14)	2.5(13)
C21	31.1(14)	15.0(13)	21.8(14)	-6.2(11)	-9.2(12)	-1.1(11)
C22	21.3(13)	19.0(14)	22.8(14)	-7.3(11)	-7.8(11)	2.8(11)
C23	22.4(13)	20.9(14)	23.7(14)	-8.2(12)	-8.4(12)	1.4(11)
C24	38.5(16)	20.4(15)	24.0(15)	-4.9(12)	-15.6(13)	-0.6(12)
C25	35.0(16)	18.1(15)	29.3(16)	-5.1(12)	-13.2(14)	1.1(12)
C26	24.6(14)	19.5(15)	36.1(17)	-13.3(13)	-11.3(13)	1.2(11)
C27	32.0(15)	25.3(16)	37.3(17)	-11.7(13)	-21.8(14)	4.6(12)
C28	31.1(15)	19.3(14)	31.8(16)	-6.1(12)	-17.8(13)	3.5(12)
C29	31.7(16)	27.8(17)	42.3(19)	-18.4(15)	-9.1(15)	1.0(13)
C30	56(2)	24.2(16)	31.9(17)	-12.2(13)	-23.6(16)	-0.2(14)
O16	46.5(14)	37.8(15)	40.5(14)	-10.4(11)	-19.1(12)	1.5(11)
C31	57(2)	40(2)	41(2)	-14.9(17)	-27.3(18)	3.5(17)

Tble S3. Bond Lengths for fa-asng.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ag1	C1	2.215(2)	O15	N5	1.208(3)
Ag1	C11	2.206(3)	N1	C6	1.476(4)
Ag2	O10	2.359(2)	N2	C16	1.476(4)
Ag2	O14	2.668(3)	N3	C26	1.472(4)
Ag2	O14 ¹	2.414(2)	C1	C2	1.448(3)
Ag2	C21	2.233(3)	C2	C3	1.508(4)
S1	C1	1.758(3)	C3	C4	1.397(4)
S1	C9	1.790(3)	C3	C8	1.390(4)
S1	C10	1.794(3)	C4	C5	1.381(4)
S2	C11	1.758(2)	C5	C6	1.382(4)
S2	C19	1.795(3)	C6	C7	1.377(4)
S2	C20	1.786(3)	C7	C8	1.383(4)
S3	C21	1.759(3)	C11	C12	1.449(4)
S3	C29	1.799(3)	C12	C13	1.519(4)
S3	C30	1.789(3)	C13	C14	1.389(4)
O1	C2	1.234(3)	C13	C18	1.384(4)
O2	N1	1.214(4)	C14	C15	1.391(4)
O3	N1	1.226(4)	C15	C16	1.372(4)
O4	C12	1.236(3)	C16	C17	1.376(4)
O5	N2	1.195(4)	C17	C18	1.387(4)
O6	N2	1.196(3)	C21	C22	1.437(4)
O7	C22	1.240(3)	C22	C23	1.508(4)
O8	N3	1.223(3)	C23	C24	1.400(4)
O9	N3	1.234(3)	C23	C28	1.388(4)
O10	N4	1.256(3)	C24	C25	1.384(4)
O11	N4	1.242(3)	C25	C26	1.378(4)
O12	N4	1.244(3)	C26	C27	1.379(4)
O13	N5	1.234(3)	C27	C28	1.379(4)
O14	Ag2 ¹	2.414(2)	O16	C31	1.396(4)
O14	N5	1.259(3)			

¹1-X,-Y,1-Z

Table S4. Bond Angles for fa-asng.

Atom	Atom	Atom	Angle/ [°]	Atom	Atom	Atom	Angle/ [°]
C11	Ag1	C1	166.14(9)	C8	C3	C2	121.5(2)
O10	Ag2	O14	106.76(8)	C8	C3	C4	119.9(2)
O10	Ag2	O14 ¹	78.88(8)	C5	C4	C3	120.0(3)
O14 ¹	Ag2	O14	69.54(11)	C4	C5	C6	118.3(3)
C21	Ag2	O10	142.08(9)	C5	C6	N1	118.4(3)
C21	Ag2	O14 ¹	133.70(9)	C7	C6	N1	118.4(3)
C21	Ag2	O14	103.74(9)	C7	C6	C5	123.2(3)
C1	S1	C9	101.50(13)	C6	C7	C8	117.9(3)
C1	S1	C10	104.26(13)	C7	C8	C3	120.6(3)
C9	S1	C10	100.68(14)	S2	C11	Ag1	112.06(13)
C11	S2	C19	102.82(13)	C12	C11	Ag1	99.61(16)
C11	S2	C20	104.45(13)	C12	C11	S2	111.58(19)
C20	S2	C19	98.68(14)	O4	C12	C11	124.2(2)
C21	S3	C29	105.29(14)	O4	C12	C13	118.3(2)
C21	S3	C30	101.69(14)	C11	C12	C13	117.5(2)
C30	S3	C29	100.41(16)	C14	C13	C12	117.5(2)
N4	O10	Ag2	109.49(18)	C18	C13	C12	123.4(2)
Ag2 ¹	O14	Ag2	110.46(11)	C18	C13	C14	119.1(3)
N5	O14	Ag2	100.61(19)	C13	C14	C15	120.9(3)
N5	O14	Ag2 ¹	118.19(19)	C16	C15	C14	117.8(3)
O2	N1	O3	124.0(3)	C15	C16	N2	118.3(3)
O2	N1	C6	118.3(3)	C15	C16	C17	123.2(3)
O3	N1	C6	117.7(3)	C17	C16	N2	118.5(3)
O5	N2	O6	122.9(3)	C16	C17	C18	117.8(3)
O5	N2	C16	118.5(3)	C13	C18	C17	121.1(3)
O6	N2	C16	118.5(3)	S3	C21	Ag2	107.01(13)
O8	N3	O9	123.7(3)	C22	C21	Ag2	105.57(18)
O8	N3	C26	118.2(3)	C22	C21	S3	111.5(2)
O9	N3	C26	118.1(3)	O7	C22	C21	122.6(2)
O11	N4	O10	119.4(3)	O7	C22	C23	119.5(2)
O11	N4	O12	120.9(3)	C21	C22	C23	117.8(2)
O12	N4	O10	119.6(3)	C24	C23	C22	123.4(2)
O13	N5	O14	117.0(3)	C28	C23	C22	117.8(2)
O15	N5	O13	122.4(3)	C28	C23	C24	118.7(3)
O15	N5	O14	120.5(3)	C25	C24	C23	120.9(3)
S1	C1	Ag1	106.22(12)	C26	C25	C24	118.3(3)
C2	C1	Ag1	99.95(16)	C25	C26	N3	119.3(3)
C2	C1	S1	112.85(19)	C25	C26	C27	122.4(3)
O1	C2	C1	124.9(2)	C27	C26	N3	118.4(3)
O1	C2	C3	118.7(2)	C26	C27	C28	118.6(3)
C1	C2	C3	116.4(2)	C27	C28	C23	121.0(3)

C4 C3 C2

118.4(2)

¹1-X,-Y,1-Z

Table S5. Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for fa-asng.

Atom	x	y	z	U(eq)
H1	587	3919	2273	23
H4	1664	2451	-93	29
H5	754	591	352	33
H7	-1797	887	2906	28
H8	-814	2705	2501	24
H9A	975	5428	2949	41
H9B	1336	6779	2350	41
H9C	2383	5913	2234	41
H10A	-626	5976	1125	46
H10B	-396	6933	1549	46
H10C	-827	5626	2280	46
H11	4815	2380	1610	23
H14	4845	2736	-1377	33
H15	3909	1174	-1500	36
H17	2981	-516	1471	36
H18	3892	1062	1585	34
H19A	6629	2497	2053	40
H19B	7746	3503	1461	40
H19C	7474	2717	901	40
H20A	4774	4968	2068	46
H20B	6062	4844	2211	46
H20C	5046	3756	2717	46
H21	2309	1915	5557	27
H24	2486	217	5246	33
H25	1700	-1476	5216	34
H27	852	398	2855	34
H28	1554	2087	2938	32
H29A	1222	4357	4903	51
H29B	1639	4940	5540	51
H29C	1090	3616	6019	51
H30A	2901	2954	6565	52
H30B	3584	4228	6119	52
H30C	4335	3204	5845	52
H16	6130(40)	1560(40)	6970(30)	62
H31A	6745	3159	5820	64
H31B	7207	3607	6512	64
H31C	5761	3315	6817	64