Supporting Information

Synthesis from Caffeine of a Mixed *N*- Heterocyclic Carbene-Silver Acetate Complex Active Against Resistant Respiratory Pathogens

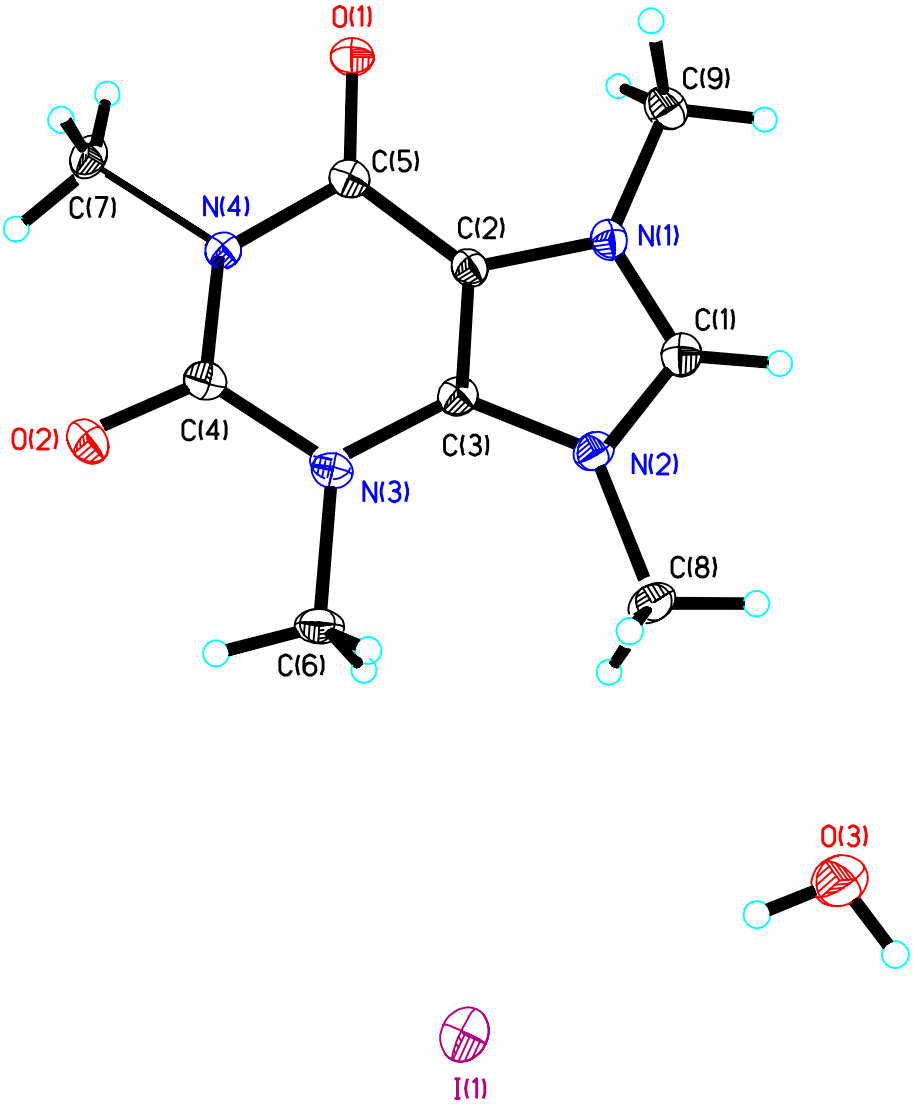
Aysegul Kascatan-Nebioglu, Abdulkareem Melaiye, Khadijah Hindi, Semih Durmus, Matthew J. Panzner, Lisa A. Hogue, Rebekah J. Mallett, Christine E. Hovis, Marvin Coughenour, Seth D. Crosby, Amy Milsted, Daniel L. Ely, Claire A. Tessier, Carolyn L. Cannon, and Wiley J. Youngs

Content:

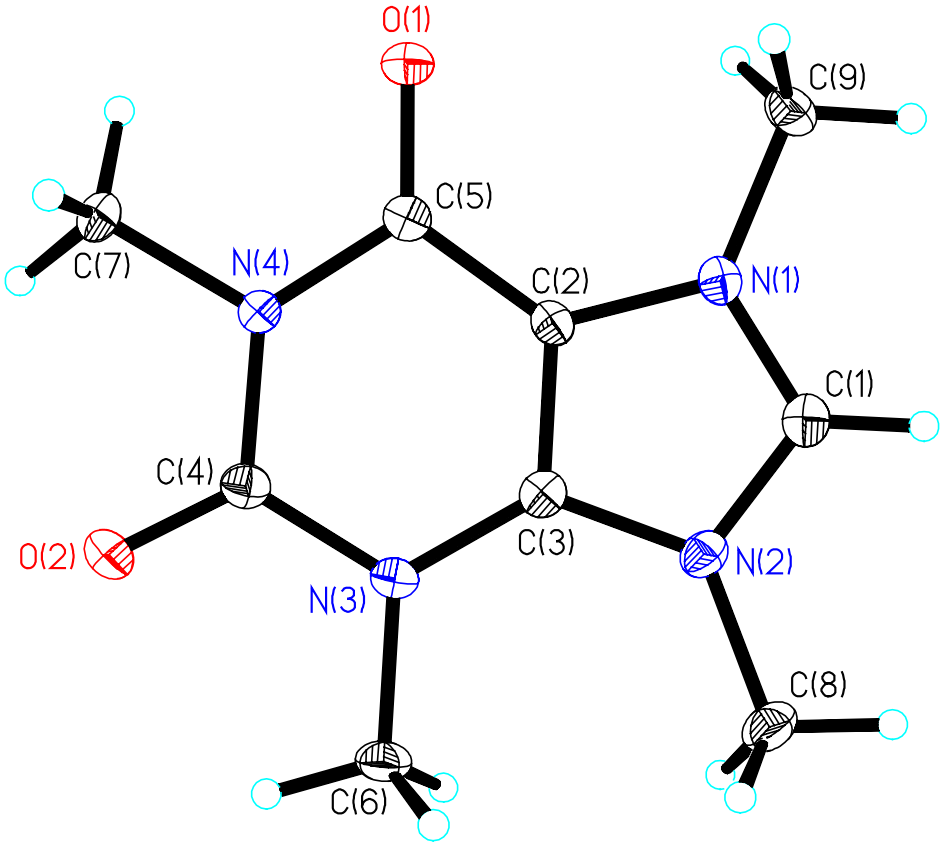
Melting Point and Elemental Analysis Table S2
Thermal Ellipsoid Plots for Compound 1 ..... S3- S5
Tables for Crystal Structure of Compound 1 ..... S6- S10
Thermal Ellipsoid Plots for Complex 3 ..... S11- S13
Tables for Crystal Structure of Complex 3 ..... S14- S22
Thermal Ellipsoid Plots for Complex 4 ..... S23- S25
Tables for Crystal Structure of Complex 4 ..... S26- S31

Compound	Melting Point	Elemental Analysis (C, H, N %)	
		Calcd	**Found**
1·H_2O	187- 190	30.52, 4.27, 15.82	30.27, 4.18, 15.41
3	120-123	40.08, 4.54, 18.70.	39.39, 4.57, 19.06
4·2H_2O	209- 212	32.11, 4.62, 13.62	31.95, 4.33, 13.18

Asymmetric Unit of 1



Molecule 1



Molecule 1 – Hydrogens Omitted

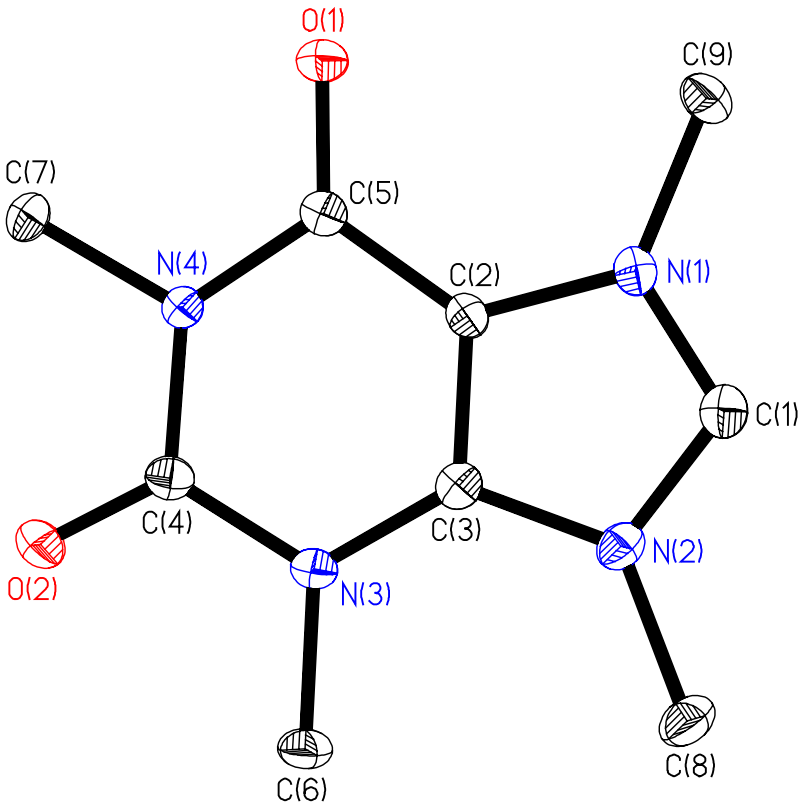


Table 1. Crystal data and structure refinement for **$C_9H_{13}N_4O_2I$, H_2O**.

Identification code	**1**	
Empirical formula	$C_9 H_{15} I N_4 O_3$	
Formula weight	354.15	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.8807(5) Å	α= 96.4480(10)°.
	b = 8.1331(6) Å	β= 99.4090(10)°.
	c = 10.8982(7) Å	γ = 110.5710(10)°.
Volume	634.19(7) $Å^3$	
Z	2	
Density (calculated)	1.855 Mg/m^3	
Absorption coefficient	2.529 mm^{-1}	
F(000)	348	
Crystal size	0.40 x 0.40 x 0.30 mm^3	
Theta range for data collection	1.93 to 28.27°.	
Index ranges	$-10 \leq h \leq 10$, $-10 \leq k \leq 10$, $-14 \leq l \leq 14$	
Reflections collected	5638	
Independent reflections	2944 [R(int) = 0.0123]	
Completeness to theta = 26.30°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5467 and 0.4311	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2944 / 0 / 166	
Goodness-of-fit on F^2	1.090	
Final R indices [I>2sigma(I)]	R1 = 0.0148, wR2 = 0.0372	
R indices (all data)	R1 = 0.0152, wR2 = 0.0374	
Largest diff. peak and hole	0.465 and -0.291 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
I(1)	6827(1)	1994(1)	3494(1)	19(1)
O(1)	-3118(2)	5739(2)	1188(1)	18(1)
O(2)	-1189(2)	1174(2)	205(1)	22(1)
O(3)	8301(2)	6531(2)	5205(1)	29(1)
N(1)	781(2)	7800(2)	2748(1)	14(1)
N(2)	2884(2)	6598(2)	2916(1)	15(1)
N(3)	959(2)	3681(2)	1512(1)	15(1)
N(4)	-2097(2)	3500(2)	633(1)	13(1)
C(1)	2507(2)	8055(2)	3264(1)	16(1)
C(2)	-28(2)	6094(2)	2027(1)	13(1)
C(3)	1286(2)	5351(2)	2132(1)	13(1)
C(4)	-806(2)	2680(2)	759(1)	15(1)
C(5)	-1870(2)	5170(2)	1284(1)	13(1)
C(6)	2384(2)	2888(2)	1593(2)	19(1)
C(7)	-3972(2)	2372(2)	-107(2)	17(1)
C(8)	4685(2)	6484(2)	3419(2)	20(1)
C(9)	-115(2)	9090(2)	2937(2)	20(1)

Table 3. Bond lengths [Å] and angles [°] for **1**.

O(1)-C(5)	1.2205(18)
O(2)-C(4)	1.2125(19)
N(1)-C(1)	1.317(2)
N(1)-C(2)	1.3849(18)
N(1)-C(9)	1.4701(19)
N(2)-C(1)	1.349(2)
N(2)-C(3)	1.3784(19)
N(2)-C(8)	1.4743(19)
N(3)-C(3)	1.3630(19)
N(3)-C(4)	1.397(2)
N(3)-C(6)	1.4748(18)
N(4)-C(5)	1.3966(19)
N(4)-C(4)	1.3972(18)
N(4)-C(7)	1.4719(19)
C(2)-C(3)	1.367(2)
C(2)-C(5)	1.429(2)
C(1)-N(1)-C(2)	107.49(13)
C(1)-N(1)-C(9)	125.67(13)
C(2)-N(1)-C(9)	126.82(13)
C(1)-N(2)-C(3)	106.90(13)
C(1)-N(2)-C(8)	121.99(13)
C(3)-N(2)-C(8)	130.97(13)
C(3)-N(3)-C(4)	118.42(12)
C(3)-N(3)-C(6)	123.09(13)
C(4)-N(3)-C(6)	118.49(12)
C(5)-N(4)-C(4)	126.50(12)
C(5)-N(4)-C(7)	116.82(12)
C(4)-N(4)-C(7)	115.95(12)
N(1)-C(1)-N(2)	110.77(13)
C(3)-C(2)-N(1)	107.44(13)
C(3)-C(2)-C(5)	122.77(13)
N(1)-C(2)-C(5)	129.79(13)
N(3)-C(3)-C(2)	122.74(13)
N(3)-C(3)-N(2)	129.84(13)
C(2)-C(3)-N(2)	107.40(13)
O(2)-C(4)-N(3)	121.41(14)
O(2)-C(4)-N(4)	121.09(14)
N(3)-C(4)-N(4)	117.47(13)
O(1)-C(5)-N(4)	122.48(14)
O(1)-C(5)-C(2)	125.73(14)
N(4)-C(5)-C(2)	111.77(12)

Symmetry transformations used to generate equivalent atoms:

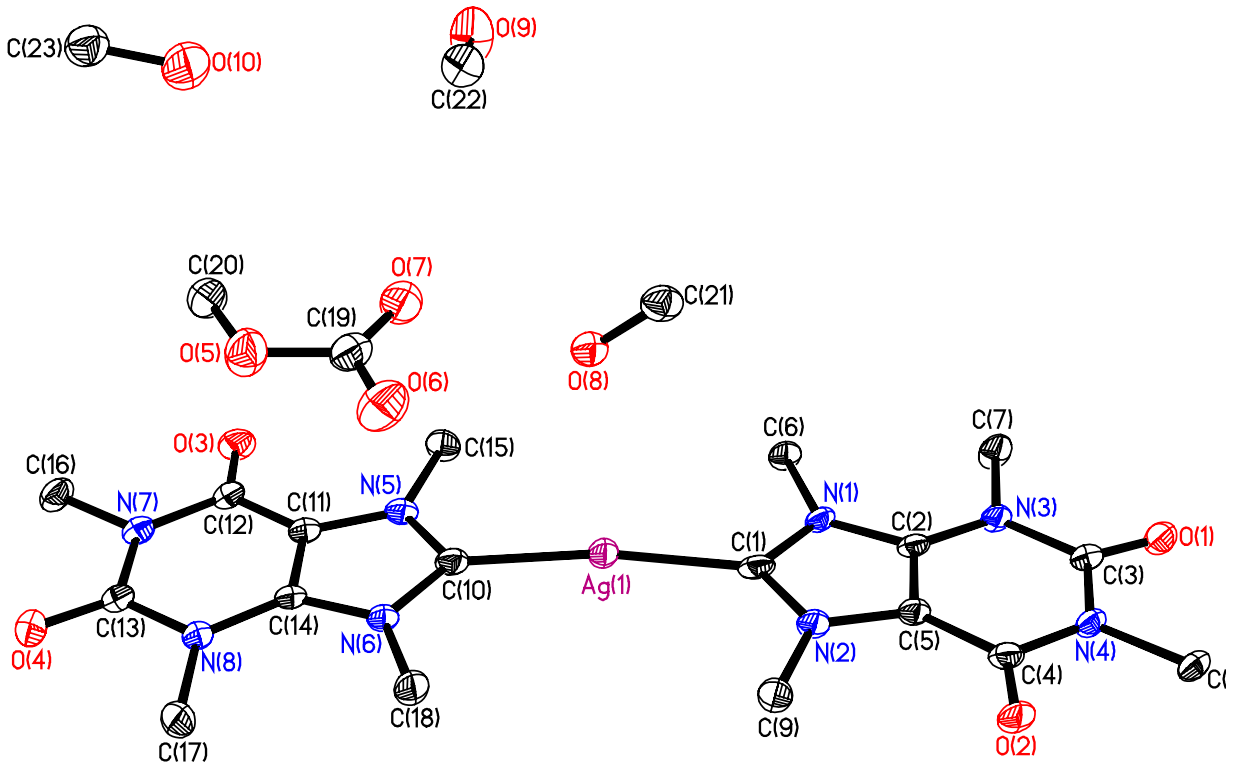
Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	18(1)	20(1)	17(1)	5(1)	4(1)	4(1)
O(1)	16(1)	18(1)	20(1)	2(1)	2(1)	9(1)
O(2)	22(1)	16(1)	26(1)	-3(1)	1(1)	10(1)
O(3)	20(1)	25(1)	38(1)	1(1)	2(1)	8(1)
N(1)	15(1)	13(1)	14(1)	1(1)	3(1)	4(1)
N(2)	12(1)	18(1)	14(1)	3(1)	3(1)	5(1)
N(3)	14(1)	15(1)	17(1)	2(1)	3(1)	8(1)
N(4)	12(1)	13(1)	14(1)	1(1)	2(1)	5(1)
C(1)	16(1)	16(1)	15(1)	3(1)	5(1)	4(1)
C(2)	14(1)	12(1)	14(1)	2(1)	4(1)	5(1)
C(3)	13(1)	15(1)	13(1)	4(1)	5(1)	4(1)
C(4)	16(1)	16(1)	15(1)	3(1)	4(1)	8(1)
C(5)	15(1)	14(1)	13(1)	4(1)	5(1)	6(1)
C(6)	15(1)	19(1)	26(1)	4(1)	5(1)	11(1)
C(7)	13(1)	16(1)	17(1)	0(1)	-1(1)	4(1)
C(8)	13(1)	26(1)	20(1)	2(1)	1(1)	8(1)
C(9)	21(1)	14(1)	26(1)	1(1)	5(1)	8(1)

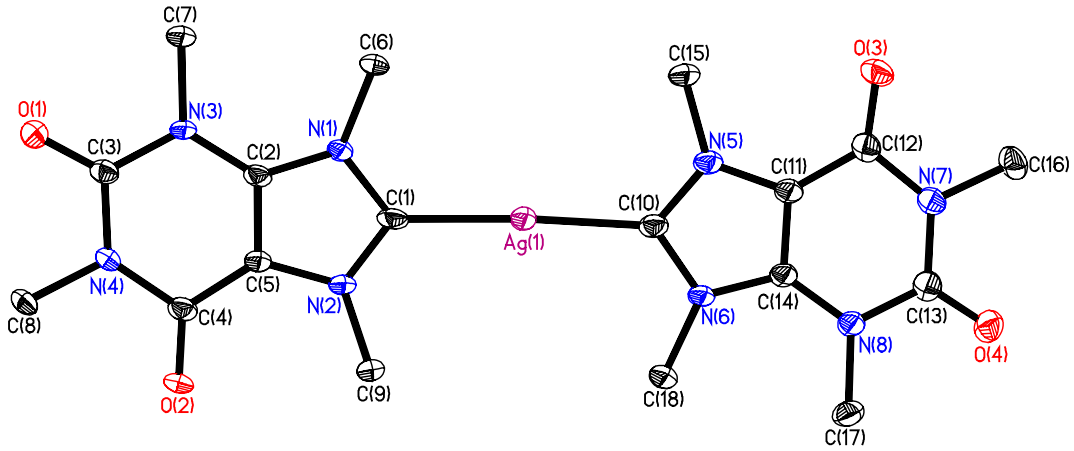
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(6)	3369	9120	3808	19
H(6A)	2750	2749	2467	28
H(6B)	3471	3671	1330	28
H(6C)	1877	1715	1036	28
H(7B)	-4684	1655	436	25
H(7C)	-3879	1579	-817	25
H(7A)	-4601	3132	-431	25
H(8A)	5491	7598	4000	30
H(8B)	5274	6297	2719	30
H(8C)	4487	5482	3874	30
H(9A)	796	10209	3461	30
H(9B)	-1139	8600	3361	30
H(9C)	-600	9321	2115	30
H(3A)	9420(40)	6860(40)	5490(30)	49(8)
H(3B)	8000(40)	5560(40)	4780(30)	53(8)

Asymmetric Unit of 3



Cationic Portion of 3



Anion

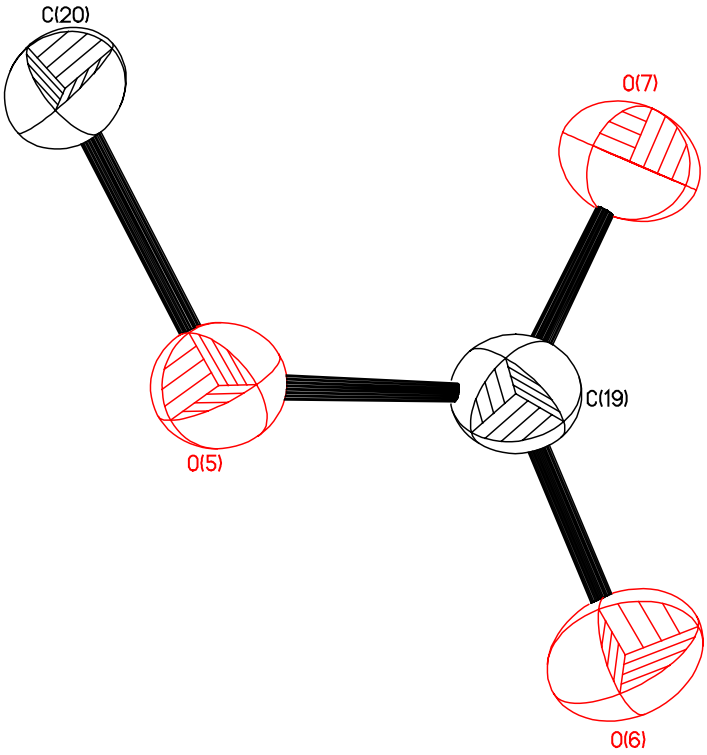


Table 1. Crystal data and structure refinement for **$C_{20}H_{27}AgN_8O_7$, $3CH_3OH$**.

Identification code	3	
Empirical formula	C_{23} H_{39} Ag N_8 O_{10}	
Formula weight	695.49	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0385(10) Å	α= 88.876(2)°.
	b = 9.1589(12) Å	β= 78.611(2)°.
	c = 20.262(3) Å	γ = 75.225(2)°.
Volume	1413.3(3) $Å^3$	
Z	2	
Density (calculated)	1.634 Mg/m^3	
Absorption coefficient	0.783 mm^{-1}	
F(000)	720	
Crystal size	0.33 x 0.28 x 0.08 mm^3	
Theta range for data collection	2.05 to 28.34°.	
Index ranges	$-10 \leq h \leq 10$, $-12 \leq k \leq 11$, $-27 \leq l \leq 27$	
Reflections collected	12637	
Independent reflections	6599 [R(int) = 0.0342]	
Completeness to theta = 26.30°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9400 and 0.7822	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6599 / 0 / 394	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0568, wR2 = 0.1464	
R indices (all data)	R1 = 0.0638, wR2 = 0.1512	
Largest diff. peak and hole	2.330 and -1.920 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	9519(1)	7282(1)	7483(1)	21(1)
O(1)	7472(4)	13923(3)	10099(1)	24(1)
O(2)	12612(3)	10332(3)	9430(1)	23(1)
O(3)	6891(4)	4345(4)	5346(2)	27(1)
O(4)	12258(4)	1067(3)	4638(2)	29(1)
O(5)	8708(5)	1587(4)	6892(2)	38(1)
O(6)	9842(5)	2662(4)	7594(2)	43(1)
O(7)	6979(5)	3547(4)	7561(2)	40(1)
O(8)	6500(4)	6376(3)	8093(2)	28(1)
O(9)	713(5)	4735(4)	8266(2)	48(1)
O(10)	3020(5)	868(5)	7028(2)	52(1)
N(1)	7990(4)	10074(4)	8488(2)	18(1)
N(2)	10740(4)	9099(4)	8477(2)	19(1)
N(3)	7464(4)	12127(4)	9337(2)	18(1)
N(4)	10021(4)	12132(4)	9758(2)	18(1)
N(5)	8565(4)	5636(4)	6347(2)	20(1)
N(6)	11330(4)	4788(4)	6355(2)	19(1)
N(7)	9576(4)	2670(4)	5015(2)	23(1)
N(8)	12069(4)	2807(4)	5450(2)	22(1)
C(1)	9426(5)	8945(4)	8195(2)	20(1)
C(2)	8445(5)	10904(4)	8938(2)	17(1)
C(3)	8259(5)	12804(4)	9752(2)	18(1)
C(4)	11094(5)	10858(4)	9374(2)	19(1)
C(5)	10183(5)	10299(4)	8942(2)	18(1)
C(6)	6276(5)	10252(5)	8302(2)	23(1)

C(7)	5588(5)	12766(5)	9355(2)	26(1)
C(8)	10823(5)	12854(5)	10207(2)	23(1)
C(9)	12540(5)	8148(5)	8313(2)	24(1)
C(10)	9824(5)	5822(4)	6663(2)	20(1)
C(11)	9236(5)	4491(4)	5861(2)	20(1)
C(12)	8408(5)	3889(4)	5407(2)	21(1)
C(13)	11347(5)	2121(5)	5015(2)	23(1)
C(14)	10978(5)	3953(4)	5872(2)	18(1)
C(15)	6729(5)	6474(5)	6526(2)	25(1)
C(16)	8843(6)	1903(5)	4554(2)	27(1)
C(17)	13959(5)	2307(5)	5415(2)	27(1)
C(18)	12985(5)	4632(5)	6576(2)	28(1)
C(19)	8465(6)	2687(5)	7380(2)	32(1)
C(20)	7238(6)	1527(5)	6611(2)	31(1)
C(21)	6403(6)	6353(5)	8799(2)	29(1)
C(22)	2356(6)	3969(5)	8397(2)	32(1)
C(23)	2918(7)	-307(6)	6598(3)	39(1)

Table 3. Bond lengths [Å] and angles [°] for **3**.

Ag(1)-C(10)	2.091(4)	N(5)-C(11)	1.380(5)
Ag(1)-C(1)	2.096(4)	N(5)-C(15)	1.456(5)
O(1)-C(3)	1.211(5)	N(6)-C(14)	1.368(5)
O(2)-C(4)	1.219(5)	N(6)-C(10)	1.375(5)
O(3)-C(12)	1.215(5)	N(6)-C(18)	1.459(5)
O(4)-C(13)	1.224(5)	N(7)-C(13)	1.384(5)
O(5)-C(19)	1.377(6)	N(7)-C(12)	1.402(5)
O(5)-C(20)	1.422(6)	N(7)-C(16)	1.473(5)
O(6)-C(19)	1.260(6)	N(8)-C(14)	1.368(5)
O(7)-C(19)	1.241(6)	N(8)-C(13)	1.385(5)
O(8)-C(21)	1.418(5)	N(8)-C(17)	1.459(5)
O(9)-C(22)	1.401(5)	C(2)-C(5)	1.367(5)
O(10)-C(23)	1.426(6)	C(4)-C(5)	1.422(5)
N(1)-C(2)	1.358(5)	C(11)-C(14)	1.365(5)
N(1)-C(1)	1.378(5)	C(11)-C(12)	1.429(5)
N(1)-C(6)	1.468(5)		
N(2)-C(1)	1.334(5)	C(10)-Ag(1)-C(1)	170.83(15)
N(2)-C(5)	1.387(5)	C(19)-O(5)-C(20)	117.7(4)
N(2)-C(9)	1.463(5)	C(2)-N(1)-C(1)	110.0(3)
N(3)-C(2)	1.364(5)	C(2)-N(1)-C(6)	129.0(3)
N(3)-C(3)	1.392(5)	C(1)-N(1)-C(6)	121.0(3)
N(3)-C(7)	1.465(5)	C(1)-N(2)-C(5)	111.0(3)
N(4)-C(3)	1.395(5)	C(1)-N(2)-C(9)	124.9(3)
N(4)-C(4)	1.403(5)	C(5)-N(2)-C(9)	124.1(3)
N(4)-C(8)	1.469(5)	C(2)-N(3)-C(3)	119.3(3)
N(5)-C(10)	1.345(5)	C(2)-N(3)-C(7)	123.0(3)
		C(3)-N(3)-C(7)	117.7(3)
		C(3)-N(4)-C(4)	126.7(3)

C(3)-N(4)-C(8)	116.0(3)	N(4)-C(4)-C(5)	111.8(3)
C(4)-N(4)-C(8)	117.3(3)	C(2)-C(5)-N(2)	106.0(3)
C(10)-N(5)-C(11)	110.7(3)	C(2)-C(5)-C(4)	123.0(4)
C(10)-N(5)-C(15)	124.2(3)	N(2)-C(5)-C(4)	131.0(3)
C(11)-N(5)-C(15)	125.1(3)	N(5)-C(10)-N(6)	105.3(3)
C(14)-N(6)-C(10)	110.3(3)	N(5)-C(10)-Ag(1)	127.2(3)
C(14)-N(6)-C(18)	128.5(3)	N(6)-C(10)-Ag(1)	127.4(3)
C(10)-N(6)-C(18)	121.1(3)	C(14)-C(11)-N(5)	106.9(3)
C(13)-N(7)-C(12)	126.7(3)	C(14)-C(11)-C(12)	122.3(4)
C(13)-N(7)-C(16)	116.8(3)	N(5)-C(11)-C(12)	130.8(4)
C(12)-N(7)-C(16)	116.6(3)	O(3)-C(12)-N(7)	121.9(4)
C(14)-N(8)-C(13)	118.1(3)	O(3)-C(12)-C(11)	126.3(4)
C(14)-N(8)-C(17)	123.7(3)	N(7)-C(12)-C(11)	111.7(3)
C(13)-N(8)-C(17)	118.2(3)	O(4)-C(13)-N(7)	121.2(4)
N(2)-C(1)-N(1)	105.5(3)	O(4)-C(13)-N(8)	120.8(4)
N(2)-C(1)-Ag(1)	126.9(3)	N(7)-C(13)-N(8)	118.1(3)
N(1)-C(1)-Ag(1)	127.5(3)	C(11)-C(14)-N(6)	106.8(3)
N(1)-C(2)-N(3)	130.4(3)	C(11)-C(14)-N(8)	123.0(4)
N(1)-C(2)-C(5)	107.6(3)	N(6)-C(14)-N(8)	130.2(3)
N(3)-C(2)-C(5)	122.1(3)	O(7)-C(19)-O(6)	128.2(5)
O(1)-C(3)-N(3)	122.2(3)	O(7)-C(19)-O(5)	118.6(4)
O(1)-C(3)-N(4)	120.7(3)	O(6)-C(19)-O(5)	113.1(4)
N(3)-C(3)-N(4)	117.0(3)		
O(2)-C(4)-N(4)	121.5(4)		
O(2)-C(4)-C(5)	126.6(4)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	14(1)	23(1)	26(1)	-7(1)	-2(1)	-6(1)
O(1)	19(1)	22(1)	30(2)	-5(1)	-3(1)	-6(1)
O(2)	11(1)	29(2)	31(2)	-5(1)	-5(1)	-6(1)
O(3)	18(1)	35(2)	31(2)	0(1)	-7(1)	-11(1)
O(4)	28(2)	26(2)	32(2)	-9(1)	-2(1)	-10(1)
O(5)	31(2)	37(2)	47(2)	-8(2)	-9(2)	-7(2)
O(6)	40(2)	43(2)	54(2)	2(2)	-19(2)	-16(2)
O(7)	31(2)	36(2)	52(2)	-10(2)	0(2)	-10(2)
O(8)	24(2)	28(2)	31(2)	-2(1)	-2(1)	-9(1)
O(9)	30(2)	48(2)	63(2)	-14(2)	-24(2)	5(2)
O(10)	37(2)	59(3)	64(3)	-12(2)	-6(2)	-22(2)
N(1)	11(1)	19(2)	25(2)	-3(1)	-2(1)	-6(1)
N(2)	10(1)	21(2)	24(2)	-3(1)	-2(1)	-3(1)
N(3)	8(1)	20(2)	26(2)	-4(1)	-2(1)	-3(1)
N(4)	13(2)	20(2)	23(2)	-2(1)	-5(1)	-7(1)
N(5)	13(2)	23(2)	24(2)	-1(1)	-1(1)	-6(1)
N(6)	11(1)	22(2)	24(2)	-3(1)	-2(1)	-6(1)
N(7)	19(2)	26(2)	26(2)	-3(1)	-3(1)	-12(1)
N(8)	16(2)	23(2)	26(2)	-6(1)	0(1)	-9(1)
C(1)	10(2)	24(2)	27(2)	2(2)	-2(1)	-7(2)
C(2)	11(2)	20(2)	22(2)	1(1)	-2(1)	-8(1)
C(3)	14(2)	20(2)	21(2)	2(1)	-3(1)	-7(1)
C(4)	14(2)	24(2)	22(2)	1(2)	-2(1)	-8(2)
C(5)	12(2)	20(2)	22(2)	-2(1)	-2(1)	-5(1)
C(6)	10(2)	29(2)	30(2)	-6(2)	-3(1)	-6(2)

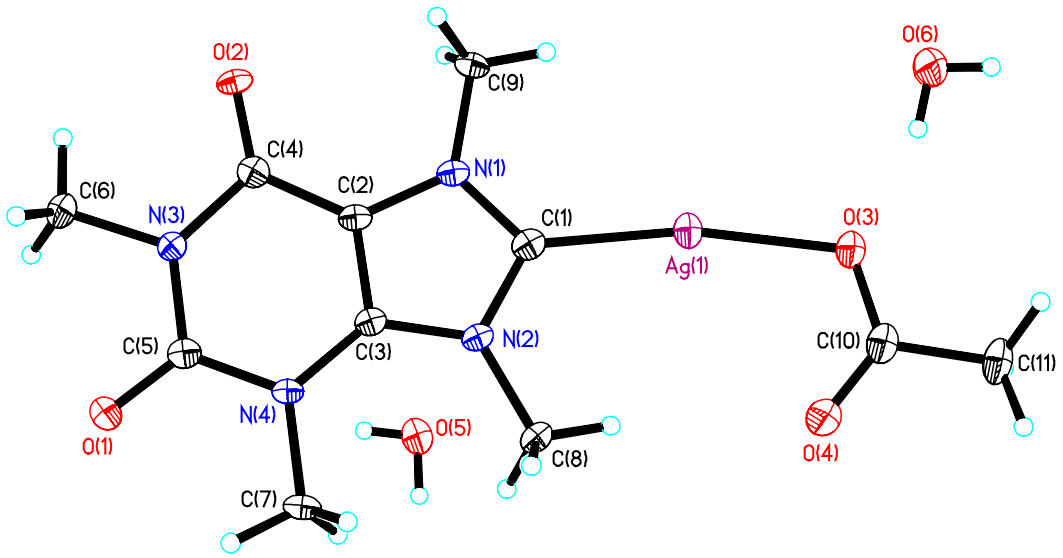
C(7)	11(2)	28(2)	40(2)	-10(2)	-6(2)	-2(2)
C(8)	17(2)	27(2)	27(2)	-6(2)	-4(2)	-11(2)
C(9)	13(2)	26(2)	30(2)	-8(2)	-2(2)	-2(2)
C(10)	13(2)	21(2)	26(2)	-1(2)	-1(1)	-6(1)
C(11)	14(2)	23(2)	24(2)	-1(2)	-2(1)	-8(2)
C(12)	21(2)	21(2)	24(2)	1(2)	-4(2)	-12(2)
C(13)	23(2)	22(2)	24(2)	-1(2)	0(2)	-13(2)
C(14)	14(2)	20(2)	22(2)	-1(1)	0(1)	-8(1)
C(15)	12(2)	29(2)	31(2)	-5(2)	-3(2)	-3(2)
C(16)	30(2)	28(2)	28(2)	-2(2)	-8(2)	-16(2)
C(17)	17(2)	24(2)	37(2)	-9(2)	-1(2)	-2(2)
C(18)	15(2)	33(2)	36(2)	-12(2)	-4(2)	-8(2)
C(19)	29(2)	32(2)	39(2)	0(2)	-5(2)	-14(2)
C(20)	30(2)	35(2)	31(2)	-2(2)	-8(2)	-12(2)
C(21)	21(2)	36(2)	31(2)	3(2)	-7(2)	-9(2)
C(22)	26(2)	31(2)	38(2)	2(2)	-11(2)	-3(2)
C(23)	34(3)	38(3)	45(3)	1(2)	-5(2)	-11(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for **3**.

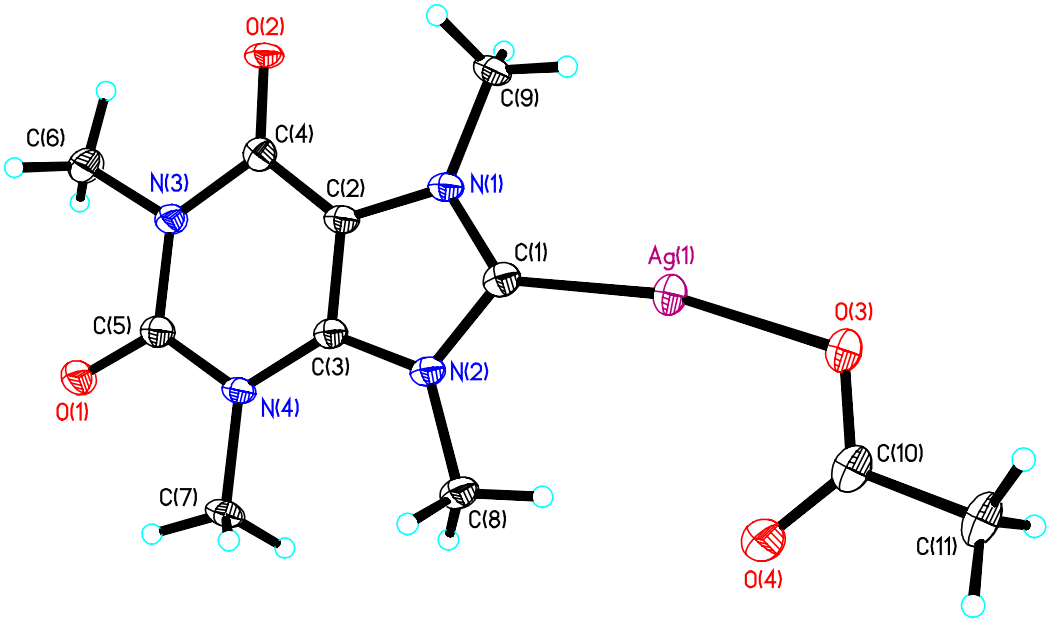
	x	y	z	U(eq)
H(8)	6752	5486	7937	42
H(9)	161	4105	8199	71
H(10)	2049	1188	7292	78
H(6A)	5403	10167	8703	34
H(6B)	6364	9462	7968	34
H(6C)	5919	11247	8110	34
H(7A)	5414	13115	8908	40
H(7B)	5141	13619	9681	40
H(7C)	4953	11991	9489	40
H(8A)	11210	13700	9981	34
H(8B)	11835	12115	10321	34
H(8C)	9959	13229	10620	34
H(9A)	12595	7315	8006	36
H(9B)	12904	7738	8727	36
H(9C)	13326	8754	8096	36
H(15A)	6036	5817	6765	37
H(15B)	6297	6820	6116	37
H(15C)	6621	7349	6818	37
H(16A)	9732	1551	4145	40
H(16B)	7815	2609	4434	40
H(16C)	8493	1036	4776	40
H(17A)	14485	3154	5294	41
H(17B)	14474	1489	5073	41
H(17C)	14189	1939	5854	41

H(18A)	13332	3637	6769	42
H(18B)	12839	5422	6918	42
H(18C)	13895	4731	6190	42
H(20A)	6409	1135	6943	47
H(20B)	7635	859	6208	47
H(20C)	6659	2544	6490	47
H(21A)	7502	5717	8897	43
H(21B)	5423	5942	9014	43
H(21C)	6217	7383	8975	43
H(22A)	3273	4021	8005	48
H(22B)	2374	2910	8485	48
H(22C)	2569	4442	8791	48
H(23A)	2639	-1140	6871	59
H(23B)	4048	-673	6288	59
H(23C)	1997	85	6340	59

Asymmetric Unit of 4



Molecule 4



Molecule 4 – Hydrogens Omitted

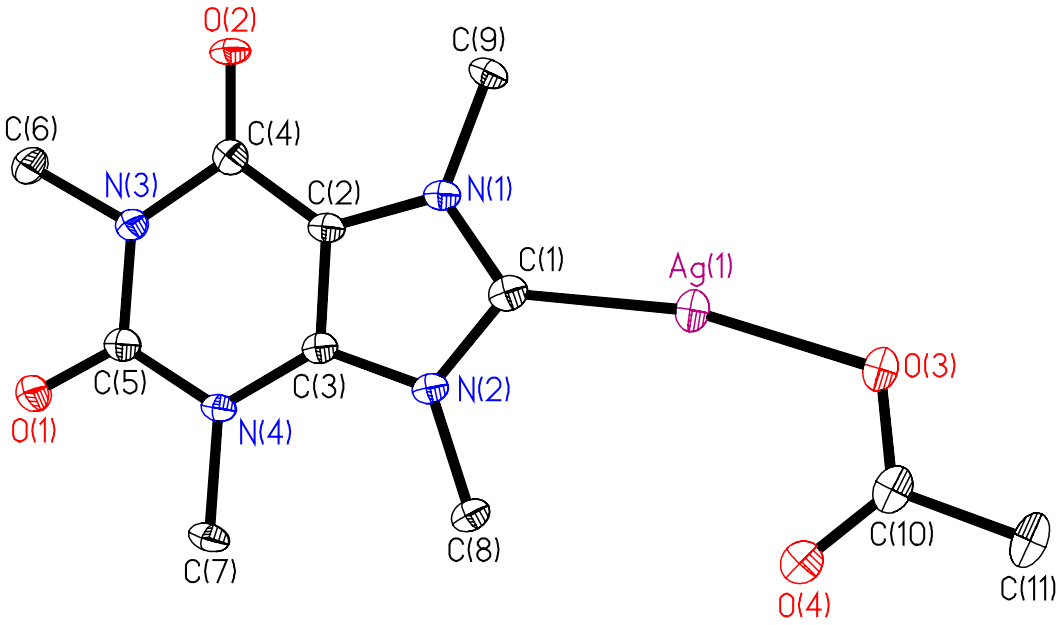


Table 1. Crystal data and structure refinement for **$C_{11}H_{15}AgN_4O_4$, 2(H_2O)**.

Identification code	**4**	
Empirical formula	C11 H19 Ag1 N4 O6	
Formula weight	411.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/m	
Unit cell dimensions	a = 8.4027(8) Å	α= 90°.
	b = 6.2961(6) Å	β= 98.243(2)°.
	c = 14.1856(14) Å	γ = 90°.
Volume	742.73(12) $Å^3$	
Z	2	
Density (calculated)	1.839 Mg/m^3	
Absorption coefficient	1.393 mm^{-1}	
F(000)	416	
Crystal size	0.21 x 0.18 x 0.03 mm^3	
Theta range for data collection	2.45 to 28.29°.	
Index ranges	$-11 \leq h \leq 10$, $-8 \leq k \leq 8$, $-18 \leq l \leq 18$	
Reflections collected	6661	
Independent reflections	1940 [R(int) = 0.0200]	
Completeness to theta = 28.29°	96.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9594 and 0.7586	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1940 / 0 / 150	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0244, wR2 = 0.0598	
R indices (all data)	R1 = 0.0256, wR2 = 0.0604	
Largest diff. peak and hole	1.593 and -0.229 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4.** U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	1015(1)	2500	5930(1)	18(1)
O(1)	888(2)	2500	474(1)	21(1)
O(2)	-3425(2)	2500	2097(1)	19(1)
O(3)	2097(2)	2500	7375(1)	21(1)
O(4)	4423(3)	2500	6794(2)	29(1)
O(5)	2274(3)	7500	3240(2)	29(1)
O(6)	-257(3)	2500	8499(2)	31(1)
N(1)	-994(3)	2500	3909(2)	15(1)
N(2)	1564(3)	2500	3846(2)	15(1)
N(3)	-1245(3)	2500	1290(2)	17(1)
N(4)	1437(3)	2500	2085(2)	15(1)
C(1)	442(3)	2500	4464(2)	17(1)
C(2)	-795(3)	2500	2957(2)	15(1)
C(3)	818(3)	2500	2925(2)	14(1)
C(4)	-1969(3)	2500	2124(2)	16(1)
C(5)	390(3)	2500	1240(2)	17(1)
C(6)	-2298(3)	2500	372(2)	22(1)
C(7)	3168(3)	2500	2035(2)	20(1)
C(8)	3306(3)	2500	4197(2)	20(1)
C(9)	-2540(3)	2500	4268(2)	19(1)
C(10)	3640(4)	2500	7475(2)	21(1)
C(11)	4478(4)	2500	8489(2)	26(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

Ag(1)-C(1)	2.067(3)
Ag(1)-O(3)	2.1198(19)
O(1)-C(5)	1.220(4)
O(2)-C(4)	1.219(3)
O(3)-C(10)	1.283(4)
O(4)-C(10)	1.244(4)
O(5)-H(5A)	0.83(5)
O(5)-H(5B)	0.74(5)
O(6)-H(6A')	0.81(6)
O(6)-H(6B')	0.85(6)
N(1)-C(1)	1.343(3)
N(1)-C(2)	1.385(3)
N(1)-C(9)	1.462(3)
N(2)-C(3)	1.366(3)
N(2)-C(1)	1.376(3)
N(2)-C(8)	1.477(3)
N(3)-C(5)	1.386(3)
N(3)-C(4)	1.406(3)
N(3)-C(6)	1.466(3)
N(4)-C(3)	1.366(3)
N(4)-C(5)	1.381(3)
N(4)-C(7)	1.466(3)
C(2)-C(3)	1.363(3)
C(2)-C(4)	1.426(4)
C(6)-H(6A)	0.9800
C(6)-H(6C)	0.9800
C(6)-H(6B)	0.9800
C(7)-H(7C)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9C)	0.9800
C(9)-H(9B)	0.9800
C(10)-C(11)	1.508(4)
C(11)-H(11C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(1)-Ag(1)-O(3)	168.19(9)
C(10)-O(3)-Ag(1)	113.15(18)
H(5A)-O(5)-H(5B)	98(4)
H(6A')-O(6)-H(6B')	105(5)
C(1)-N(1)-C(2)	110.4(2)
C(1)-N(1)-C(9)	124.3(2)
C(2)-N(1)-C(9)	125.3(2)
C(3)-N(2)-C(1)	110.3(2)
C(3)-N(2)-C(8)	128.2(2)
C(1)-N(2)-C(8)	121.5(2)
C(5)-N(3)-C(4)	126.4(2)
C(5)-N(3)-C(6)	115.6(2)
C(4)-N(3)-C(6)	118.0(2)
C(3)-N(4)-C(5)	118.8(2)
C(3)-N(4)-C(7)	123.1(2)

C(5)-N(4)-C(7)	118.1(2)	H(7C)-C(7)-H(7A)	109.5
N(1)-C(1)-N(2)	105.5(2)	H(7B)-C(7)-H(7A)	109.5
N(1)-C(1)-Ag(1)	130.6(2)	N(2)-C(8)-H(8B)	109.5
N(2)-C(1)-Ag(1)	123.99(19)	N(2)-C(8)-H(8A)	109.5
C(3)-C(2)-N(1)	107.0(2)	H(8B)-C(8)-H(8A)	109.5
C(3)-C(2)-C(4)	123.1(2)	N(2)-C(8)-H(8C)	109.5
N(1)-C(2)-C(4)	130.0(2)	H(8B)-C(8)-H(8C)	109.5
C(2)-C(3)-N(2)	106.9(2)	H(8A)-C(8)-H(8C)	109.5
C(2)-C(3)-N(4)	122.2(2)	N(1)-C(9)-H(9A)	109.5
N(2)-C(3)-N(4)	130.9(2)	N(1)-C(9)-H(9C)	109.5
O(2)-C(4)-N(3)	121.8(2)	H(9A)-C(9)-H(9C)	109.5
O(2)-C(4)-C(2)	126.7(3)	N(1)-C(9)-H(9B)	109.5
N(3)-C(4)-C(2)	111.5(2)	H(9A)-C(9)-H(9B)	109.5
O(1)-C(5)-N(4)	121.1(2)	H(9C)-C(9)-H(9B)	109.5
O(1)-C(5)-N(3)	120.9(2)	O(4)-C(10)-O(3)	123.5(3)
N(4)-C(5)-N(3)	117.9(2)	O(4)-C(10)-C(11)	120.9(3)
N(3)-C(6)-H(6A)	109.5	O(3)-C(10)-C(11)	115.5(3)
N(3)-C(6)-H(6C)	109.5	C(10)-C(11)-H(11C)	109.5
H(6A)-C(6)-H(6C)	109.5	C(10)-C(11)-H(11A)	109.5
N(3)-C(6)-H(6B)	109.5	H(11C)-C(11)-H(11A)	109.5
H(6A)-C(6)-H(6B)	109.5	C(10)-C(11)-H(11B)	109.5
H(6C)-C(6)-H(6B)	109.5	H(11C)-C(11)-H(11B)	109.5
N(4)-C(7)-H(7C)	109.5	H(11A)-C(11)-H(11B)	109.5
N(4)-C(7)-H(7B)	109.5		
H(7C)-C(7)-H(7B)	109.5		
N(4)-C(7)-H(7A)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for **4.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	21(1)	18(1)	14(1)	0	1(1)	0
O(1)	19(1)	30(1)	15(1)	0	4(1)	0
O(2)	9(1)	25(1)	23(1)	0	2(1)	0
O(3)	22(1)	25(1)	15(1)	0	0(1)	0
O(4)	21(1)	42(1)	22(1)	0	1(1)	0
O(5)	27(1)	40(1)	19(1)	0	4(1)	0
O(6)	27(1)	47(2)	19(1)	0	4(1)	0
N(1)	11(1)	16(1)	18(1)	0	3(1)	0
N(2)	11(1)	16(1)	17(1)	0	1(1)	0
N(3)	13(1)	23(1)	14(1)	0	1(1)	0
N(4)	10(1)	19(1)	17(1)	0	4(1)	0
C(1)	16(1)	14(1)	20(1)	0	1(1)	0
C(2)	12(1)	15(1)	19(1)	0	4(1)	0
C(3)	13(1)	13(1)	17(1)	0	2(1)	0
C(4)	18(1)	13(1)	18(1)	0	3(1)	0
C(5)	15(1)	18(1)	19(1)	0	3(1)	0
C(6)	18(1)	31(2)	16(1)	0	-2(1)	0
C(7)	12(1)	26(1)	23(1)	0	7(1)	0
C(8)	13(1)	27(2)	19(1)	0	-1(1)	0
C(9)	14(1)	24(1)	20(1)	0	7(1)	0
C(10)	25(1)	19(1)	19(1)	0	-2(1)	0
C(11)	32(2)	24(2)	18(1)	0	-7(1)	0

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(6A)	-2012	3692	-16	33
H(6C)	-3419	2646	479	33
H(6B)	-2165	1163	38	33
H(7C)	3342	2374	1369	30
H(7B)	3675	1297	2400	30
H(7A)	3643	3829	2302	30
H(8B)	3769	1131	4050	30
H(8A)	3478	2726	4887	30
H(8C)	3827	3643	3885	30
H(9A)	-2358	2364	4964	28
H(9C)	-3191	1303	3992	28
H(9B)	-3106	3833	4091	28
H(11C)	4535	3956	8736	38
H(11A)	5568	1932	8508	38
H(11B)	3874	1612	8882	38
H(5A)	3230(60)	7500	3150(30)	42(12)
H(6A')	40(70)	2500	9070(40)	68(17)
H(5B)	1900(60)	7500	2740(40)	45(14)
H(6B')	610(70)	2500	8250(40)	78(19)