Crystal structure of 4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo-[8.8.8]hexacosanesilver(I) nitrate, $[(C_{18}H_{36}N_2O_6)Ag]NO_3$

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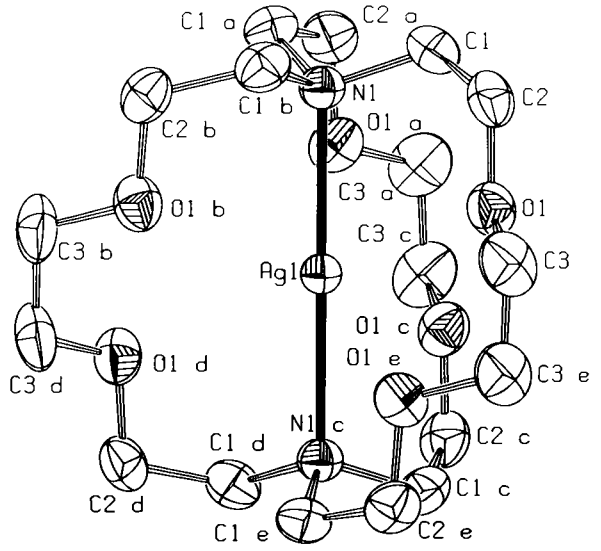

Source of material: Crystals obtained by diffusion of solutions of cryptand 222 and silver nitrate in water/methanol.
The nitrate group is disordered. Belaj et al. have determined the crystal structure of cryptand 222-silver(I) perchlorate. From powder diffraction data they deduced that the cryptand 222-silver(I) nitrate is isopointal (see ref. 1). Our measurement confirmes their statement.

$C_{18}H_{36}AgN_3O_9$, trigonal, $R\bar{3}2$ (No. 155), a =8.524(4) Å, c =27.61(2) Å, V =1737.3 Å^3, Z =3, $R(F)$ =0.038, $R_w(F)$ =0.087.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless plate, size 0.2 x 0.2 x 0.3 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.60 cm^{-1}
Diffractometer:	Siemens-Nicolet
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	55°
N(hkl)$_{unique}$:	896
Criterion for F_o:	$F_o > 4\,\sigma(F_o)$
N($param$)$_{refined}$:	49
Program:	SHELX-76

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	Occ.	x	y	z	U_{iso}
H(1A)	18*f*		-0.1467(7)	0.0279(7)	0.1407(2)	0.08
H(1B)	18*f*		-0.2574(7)	-0.0505(7)	0.0928(2)	0.08
H(2A)	18*f*		-0.2030(8)	0.2430(8)	0.1046(2)	0.08
H(2B)	18*f*		0.0071(8)	0.3174(8)	0.1062(2)	0.08
H(3A)	18*f*		-0.068(1)	0.4858(9)	0.0369(2)	0.08
H(3B)	18*f*		0.117(1)	0.4860(9)	0.0392(2)	0.08
O(2)	18*f*	0.25	0.429(4)	0.695(7)	0.2016(9)	0.16(1)
O(3)	18*f*	0.25	0.459(2)	0.824(3)	0.1582(7)	0.100(6)

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ag	3*a*	0	0	0	0.0466(2)	0.0466(2)	0.0453(2)	0.0233(1)	0	0
N(1)	6*c*	0	0	0.0874(1)	0.059(1)	0.059(1)	0.051(2)	0.0293(7)	0	0
O(1)	18*f*	-0.0986(5)	0.2402(5)	0.0413(1)	0.079(2)	0.073(2)	0.087(2)	0.046(2)	0.012(2)	0.007(2)
C(1)	18*f*	-0.1407(7)	0.0393(7)	0.1057(2)	0.077(3)	0.085(3)	0.064(2)	0.041(3)	0.014(2)	-0.003(2)
C(2)	18*f*	-0.1063(8)	0.2255(8)	0.0922(2)	0.077(3)	0.082(3)	0.086(3)	0.050(3)	0.004(2)	-0.014(2)
C(3)	18*f*	-0.005(1)	0.4244(9)	0.0257(2)	0.122(5)	0.064(3)	0.124(4)	0.059(4)	0.026(4)	0.004(3)
N(2)	3*b*	1/3	2/3	1/6	0.073(3)	0.073(3)	0.123(7)	0.037(2)	0	0

References

1. Belaj, F.; Trnoska, A.; Nachbaur, E.: Structures of cryptates Ag(C222)X and Na(C222)X. Z. Kristallogr. **212** (1997) 355-361.
2. Sheldrick, G. M.: SHELXL-76, Programs for Crystal Structures Determination. University of Cambridge, UK 1976.