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Structure of the 2,5,8-Trithia[9](2,6)pyridinophane–Silver Nitrate Complex (1:1)

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Abstract. $C_{11}H_{15}NS_3.AgNO_3$, $M_r = 427{\cdot}3$, orthorhombic, $Pca2_1$, $a = 8{\cdot}616\,(1)$, $b = 10{\cdot}303\,(2)$, $c = 16{\cdot}839\,(2)$ Å, $V = 1494{\cdot}8$ Å^3, $Z = 4$, $D_m = 1{\cdot}91$, $D_x = 1{\cdot}898$ Mg m^{-3}, $F(000) = 856$, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 1{\cdot}621$ mm^{-1}, $T = 293$ K. The structure was solved by the heavy-atom method and refined to $R = 0{\cdot}033$ and $wR = 0{\cdot}039$ for 2094 unique reflections. The Ag^+ cation sits in the cavity of the macrocycle and coordinates to three S atoms [S(4), S(7) and S(10)] and one N atom, N(1) of the pyridine ring. Ag^+ also coordinates to an S atom, S(7′) $(-0{\cdot}5 + x, -y, z)$, from an adjacent ligand. The intermolecular Ag—S interaction [2·498 (1) Å] is stronger than the intramolecular Ag—S interactions [2·701 (2), 2·710 (2) and 2·856 (1) Å]. Ag—S distances suggest covalent character of the bonds. The nitrate anion does not interact with the Ag^+ cation.

Introduction. Substitution of N or S for O in cyclic polyethers greatly influences the complexing properties. When S replaces O as a donor atom in the macrocycle the stabilities of Ag^+ and Hg^+ complexes increase while those of alkali complexes decrease (Frensdorff, 1971; Izatt, Terry, Hansen, Avondet, Bradshaw, Dalley, Jensen, Christensen & Haymore, 1978). The decrease in stability of alkali-metal complexes of polyether sulfides is probably due to the lower electronegativity, the larger size, and the different bond lengths and bond angles associated with the S atom compared to those of O. These factors tend to weaken the electrostatic attraction for alkali cations. In contrast, covalent bonding plays an important part in the Ag^+ and Hg^+ complexes. The crystal structure of the hetero analogue of '12-crown-4', namely 2,5,8-trithia[9](2,6)pyridinophane (1), has been described by Weber, Jones & Sheldrick (1983). This compound was reported to form crystalline complexes with $AgNO_3$, $HgCl_2$, $HAuCl_4$, $PdCl_2$, H_2PtCl_6 and $Co(SCN)_2$ (Weber & Vogtle, 1976). The crystal structure analysis of the title compound was undertaken to study the possible structural changes due to complexing of $AgNO_3$.

Experimental. Colourless needle shaped crystals, crystal size 0·1 × 0·1 × 0·4 mm, density measured by flotation, data collection on an automated Stoe four-circle diffractometer using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0{\cdot}71073$ Å), lattice parameters by least-squares analysis of θ values of 24 high-angle reflections in the range $20 < 2\theta < 30°$; $\omega/2\theta$ scan technique, $2\theta_{\max} = 60°$; index range: $0 \le h \le 12$, $0 \le k \le 14$, $0 \le l \le 23$; three standard reflections monitored every 100 reflections showed no significant variations; 2412 reflections measured of which 2094 reflections with $I \ge 3\sigma(I)$ considered observed; empirical absorption correction was applied using ψ scans (North, Phillips & Mathews, 1968), max. and min. transmission 1·11 and 0·83; Lorentz and polarization corrections applied. Structure was solved by heavy-atom method using *SHELX76* (Sheldrick, 1976); Ag and S positions from the Patterson map; rest of the non-H atoms from the subsequent Fourier maps; H-atom positions from difference Fourier maps; anisotropic refinement for non-H atoms and isotropic refinement for H atoms using full-matrix least-squares refinement; the isotropic temperature factors of four of the hydrogens were kept fixed at 0·05 Å^2 during refinement. Final $R = 0{\cdot}033$ and $wR = 0{\cdot}039$ for 2094 observed reflections; weighting scheme used, $w = 1{\cdot}00/[\sigma^2(F_o) + 0{\cdot}01203|F_o|^2]$, (shift/

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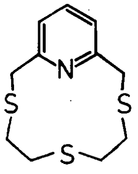
e.s.d.)$_{\max}$ in the final cycle of refinement for non-H atoms was 0·039, reflections/parameters refined ratio was 8·87; the minimum and maximum heights in the final difference Fourier map were −0·82 and +0·81 e Å^{-3}. Atomic scattering factors for non-H atoms from Cromer & Mann (1968), for H atoms from Stewart, Davidson & Simpson (1965); anomalous-dispersion correction from Cromer & Liberman (1970). Fractional coordinates and equivalent isotropic thermal parameters of the non-H atoms are given in Table 1; bond lengths and angles in Table 2.* The atom labels correspond to Fig. 1.



(1)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3) *for the non-*H *atoms, with e.s.d.'s in parentheses*

$$U_{\rm eq} = \tfrac{1}{3}\sum_{i=1}^{3} U_{ii}.$$

	x	y	z	$U_{\rm eq}$
N(1)	0·1131 (5)	0·3641 (4)	1·1592 (2)	31 (2)
C(2)	0·1539 (5)	0·4073 (5)	1·0879 (3)	33 (2)
C(3)	0·1334 (7)	0·3215 (6)	1·0156 (3)	39 (2)
S(4)	0·1510 (2)	0·1487 (1)	1·0251 (1)	35 (1)
C(5)	0·3573 (6)	0·1235 (6)	1.0324 (3)	38 (2)
C(6)	0·4334 (7)	0·1527 (5)	1·1129 (3)	36 (2)
S(7)	0·3643 (1)	0·0394 (1)	1·1888 (1)	29 (4)
C(8)	0·4365 (6)	0·1153 (6)	1·2794 (3)	32 (2)
C(9)	0·3598 (5)	0·2433 (5)	1·3012 (3)	34 (2)
S(10)	0·1553 (1)	0·2245 (1)	1·3220 (1)	34 (5)
C(11)	0·0843 (7)	0·3882 (6)	1·3039 (3)	44 (2)
C(12)	0.1287 (5)	0·4417 (5)	1·2231 (3)	39 (2)
C(13)	0·1832 (5)	0·5658 (5)	1·2160 (3)	37 (2)
C(14)	0·2236 (7)	0·6136 (6)	1·1422 (4)	46 (3)
C(15)	0·2080 (7)	0·5333 (6)	1·0771 (4)	45 (3)
Ag	0·0566 (0)	0·1411 (0)	1·1780 (0)	39 (2)
N(2)	0·2501 (7)	−0·2232 (5)	0·9148 (3)	48 (3)
O(1)	0·2527 (12)	−0·1815 (7)	0·9856 (4)	89 (5)
O(2)	0·3004 (8)	−0·3347 (6)	0·9038 (4)	69 (3)
O(3)	0·2033 (9)	−0·1614 (8)	0·8554 (6)	93 (5)

Discussion. *Structure of the macrocycle.* Fig. 1 shows the conformation of the molecule (Motherwell & Clegg, 1978). The torsion angles of the macrocycle were expected to be 180° (*anti*) for C—N—C—C and ± 60° (*gauche*) for X—C—C—X, X = N or S (Hilgenfeld & Saenger, 1982). The C—S—C—C torsion angles were grouped into two classes, those close to ± 60° (*gauche*) and those close to 180° (*anti*), as observed by Campbell, Dalley, Izatt & Lamb (1981). Starting from the N(1)—C(2) bond, the macrocycle has the conformation $ag^-g^-ggaggagga$. The endocyclic torsion angles of the macrocycle are listed in Table 2. In the title compound, the torsion angles about the C—C bonds are nearly *gauche* in contrast to that observed in its uncomplexed analogue, 2,5,8-trithia[9](2,6)pyridinophane (Weber, Jones & Sheldrick, 1983), where most of the torsion angles about the C—C bonds are *anti*. The uncomplexed analogue has the conformation $aag^-g^-ag^-gaggga$. Considerable deviations for *gauche* (± 60°) are observed for the torsion angles about the C(2)—C(3) and C(11)—C(12) bonds due to the bending of the pyridine ring away from Ag$^+$ in order to facilitate the lone pair of the pyridine N pointing towards the Ag$^+$ cation. The torsion angles about the C(5)—C(6), C(6)—S(7), S(7)—C(8) and C(8)—(9) bonds explain the folding of the ligand thus enabling S(7) to coordinate with Ag$^+$. The overall conformation of the macrocycle can be best described as a distorted half-chair as compared to the chair form observed in the uncomplexed species (Weber, Jones & Sheldrick, 1983). Bonding dimensions of the macrocycle are listed in Table 2. The C(sp^3)—C(sp^3) distances range from 1·515(8) to 1·537(7) Å with a mean of 1·523(8) Å. The shortening of C(sp^3)—C(sp^3) bond lengths in cyclic polyethers has been discussed extensively (Mercer & Truter, 1973; Dunitz, Dobler, Seiler & Phizackerley, 1974; Goldberg, 1975; Dalley, 1978; Hilgenfeld & Saenger, 1982). The C—S bond parameters are normal and are comparable with other cyclic thioethers (Campbell, Larson & Dalley, 1981*a*,*b*; Weber, Jones & Sheldrick, 1983). C(sp^2)—N bonds of the pyridine ring differ slightly and are comparable with those observed by Weber (1982) and Chacko, Ruban, Aoki & Weber (1988). The pyridine ring is planar to within 0·011(4) Å. The average C—H bond observed in the structure is 0·93(10) Å.

Cation coordination. Fig. 1 shows the coordination of the complex. The packing in the unit cell is shown in Fig. 2 (Johnson, 1965). Each Ag$^+$ cation coordinates to three S atoms [S(4), S(7) and S(10)] and one N atom, N(1) of the pyridine ring. In addition to the intramolecular Ag—S interactions, there is an Ag$^+$ interaction with the S atom S(7′) (−0·5 + x, −y, z) of an adjacent ligand (*cf.* Fig. 2). Similar intermolecular Ag—S contacts [2·673 (18) and 2·613 (18) Å] were observed in the hydrated silver nitrate complex of 1,4,7,10,13-pentaoxa-16-thiacyclooctadecane (Campbell & Dalley, 1981). In the title compound, the intermolecular Ag—S interaction [2·498(1) Å] is stronger than the intramolecular Ag—S interactions [2·701 (2)–2·856 (1) Å]. Ag—S contact distances are considerably less than the sum

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* Lists of observed and calculated structure factors, anisotropic thermal parameters for non-H atoms and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52050 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsion angles* (°) *involving non-*H *atoms, with e.s.d.'s in parentheses*

N(1)—C(2)	1·327 (6)	N(1)—C(12)	1·347 (6)
C(2)—C(3)	1·515 (8)	C(2)—C(15)	1·392 (8)
C(3)—S(4)	1·794 (6)	S(4)—C(5)	1·800 (6)
C(5)—C(6)	1·537 (7)	C(6)—S(7)	1·830 (5)
S(7)—C(8)	1·823 (6)	C(8)—C(9)	1·521 (8)
C(9)—S(10)	1·807 (4)	S(10)—C(11)	1·819 (6)
C(11)—C(12)	1·518 (7)	C(12)—C(13)	1·367 (7)
C(13)—C(14)	1·381 (8)	C(14)—C(15)	1·381 (9)
N(2)—O(1)	1·268 (9)	N(2)—O(2)	1·241 (8)
N(2)—O(3)	1·253 (11)		
Ag···N(1)	2·370 (4)	Ag···S(4)	2·701 (2)
Ag···S(7)	2·856 (1)	Ag···S(10)	2·710 (2)
Ag···S(7)′	2·498 (1)		

N(1)—C(2)—C(3)	120·0 (4)	C(2)—C(3)—S(4)	119·8 (4)
C(3)—S(4)—C(5)	103·5 (3)	S(4)—C(5)—C(6)	116·9 (4)
C(5)—C(6)—S(7)	110·6 (4)	C(6)—S(7)—C(8)	101·5 (3)
S(7)—C(8)—C(9)	115·2 (4)	C(8)—C(9)—S(10)	112·2 (4)
C(9)—S(10)—C(11)	101·3 (3)	S(10)—C(11)—C(12)	113·8 (4)
C(11)—C(12)—N(1)	118·4 (4)	C(12)—N(1)—C(2)	119·8 (3)
C(2)—C(15)—C(14)	119·2 (5)	C(15)—C(14)—C(13)	118·5 (5)
C(14)—C(13)—C(12)	119·9 (4)	C(13)—C(12)—N(1)	121·3 (4)
C(13)—C(12)—C(11)	120·3 (4)	C(15)—C(2)—N(1)	121·3 (4)
C(15)—C(2)—C(3)	118.6 (4)	O(1)—N(2)—O(2)	116·6 (5)
O(2)···Ag···S(4)	117·6 (5)	O(3)—N(2)—O(1)	125·8 (5)
N(1)···Ag···S(4)	77·5 (2)	N(1)···Ag···S(7)	100·0 (1)
N(1)···Ag···S(10)	75·4 (2)	S(4)···Ag···S(7)	78·0 (1)
S(4)···Ag···S(10)	138·6 (1)	S(7)···Ag···S(10)	76·6 (1)

N(1)—C(2)—C(3)—S(4)	− 31·7 (7)	C(2)—C(3)—S(4)—C(5)	− 76·2 (5)
C(3)—S(4)—C(5)—C(6)	77·7 (5)	S(4)—C(5)—C(6)—S(7)	65·8 (5)
C(5)—C(6)—S(7)—C(8)	− 168·3 (4)	C(6)—S(7)—C(8)—C(9)	68·3 (4)
S(7)—C(8)—C(9)—S(10)	63·2 (5)	C(8)—C(9)—S(10)—C(11)	− 157·0 (4)
C(9)—S(10)—C(11)—C(12)	53·2 (4)	S(10)—C(11)—C(12)—N(1)	44·5 (6)
C(11)—C(12)—N(1)—C(2)	− 178·6 (5)	C(12)—N(1)—C(2)—C(3)	− 178·7 (5)
C(3)—C(2)—C(15)—C(14)	178·4 (5)	C(2)—C(15)—C(14)—C(13)	− 0·7 (9)
C(15)—C(14)—C(13)—C(12)	− 0·2 (8)	C(14)—C(13)—C(12)—C(11)	179·8 (5)
C(13)—C(12)—C(11)—S(10)	− 135·4 (4)	N(1)—C(12)—C(13)—C(14)	− 0·1 (8)
N(1)—C(2)—C(15)—C(14)	2·0 (9)	C(2)—N(1)—C(12)—C(13)	1·3 (7)
C(12)—N(1)—C(2)—C(15)	− 2·2 (7)		

of their ionic and van der Waals radii, 3·11 Å (Pauling, 1960), and indicate considerable covalent character in their interactions. Ag—S contact distances are comparable with those observed by Campbell & Dalley (1981) [2·584 (17)–2·673 (18) Å], Louis, Agnus & Weiss (1977) [2·539 (2)–2·855 (2) Å] and Louis, Pelissard & Weiss (1976) [2·526 (2)–3·005 (2) Å]. The Ag—N contact distance [2·370 (4) Å] is significantly less than the sum of the ionic and van der Waals radii, 2·96 Å. The Ag^+ cation is essentially five coordinated and the geometry around Ag^+ can be best described as a highly distorted square pyramid with the hetero atoms N(1), S(4), S(7) and S(10) forming the basal plane and S(7′) occupying the apical position (Fig. 1). The basal plane is distorted with N(1) (0·3976 Å) and S(7) (0·2987 Å) lying above the mean plane and S(4) (−0·3429 Å) and S(10) (−0·3535 Å) lying below the mean plane. Due to small ring size, N(1)···S(7) = 4·016 (4), S(4)···S(10) = 5·061 (2) Å, large radii of the hetero atoms (S) and strong Ag—S(7′) interaction, Ag^+ is displaced considerably (−1·3028 Å) from the basal plane towards S(7′) thus distorting the square pyramidal geometry. S(7′) is displaced from the basal plane by −3·7192 Å. Similar Ag^+ coordination geometry is observed in the Ag(SCN) complex of 1-oxa-7,10-dithia-4,13-diazacyclopentadecane (Louis, Pelissard & Weiss, 1976).

Anion structure and interaction. The average N—O distance of the NO_3^- ion [1·254 (10) Å] is comparable to that observed in the structure of silver nitrate (1·25 Å) (Gibbons & Trotter, 1971). The nitrate ion is planar to within 0·004 (6) Å. The nitrate anion does not interact with the Ag^+ cation (Fig. 2). The shortest Ag^+ nitrate distance is 3·739 Å [Ag—O(3)(−*x*, −*y*, 0·5 + *z*)] as compared to 5·33 Å observed in the hydrated silver nitrate complex of 1,4,7,10,13-pentaoxa-16-thiacyclooctadecane (Campbell & Dalley, 1981). The nitrate ion appears to be stabilized by C—H···O type interactions, namely C(5)—H(5)···O(1) [3·362(10) Å, 159(7)°], C(13)—H(13)···O(2) (0·5 − *x*, 1 + *y*, 0·5 + *z*) [3·327 (8) Å, 147 (7)°], C(15)—H(15)···O(2) (*x*, 1 + *y*, *z*) [3·316 (9) Å, 160 (8)°] and C(8)—H(11)···O(3) (0·5 − *x*, *y*, 0·5 + *z*) [3·349 (10) Å, 140 (12)°] (compared

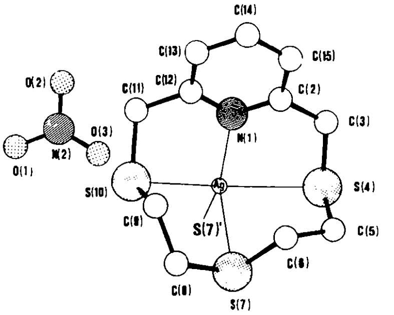

Fig. 1. Molecular structure of (1).$AgNO_3$ (1:1), viewed approximately in the crystallographic **a** direction. Hetero atoms are specified by different shading. Coordination around the cation is indicated by thin lines; S(7)′ denotes an S atom of an adjacent ligand (see Fig. 2).

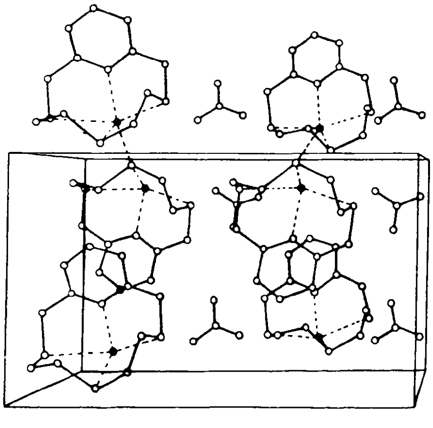

Fig. 2. Unit cell of (1).$AgNO_3$ (1:1) viewed down the crystallographic *a* axis. Ag^+ ions are specified as bold dots.

to the sum of their van der Waals radii, 3·4 Å). The geometry of C—H···O contacts is consistent with the expected spatial arrangement for a 'normal' hydrogen bond between an H atom and an orbital containing non-bonded electrons on O (Allen, Kennard & Taylor, 1983; Taylor & Kennard, 1982). S···O short contacts are also observed: O(1)···S(4) ($0{\cdot}5 + x, -y, z$) [3·512 (10) Å], O(3)···S(10) ($-x, -y, -0{\cdot}5 + z$) [3·531 (10) Å] (compared to the sum of their van der Waals radii, 3·65 Å).

The crystal packing is stabilized by van der Waals forces.

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References

ALLEN, F. H., KENNARD, O. & TAYLOR, R. (1983). *Acc. Chem. Res.* **16**, 146–153.

CAMPBELL, M. L. & DALLEY, N. K. (1981). *Acta Cryst.* **B37**, 1750–1753.

CAMPBELL, M. L., DALLEY, N. K., IZATT, R. M. & LAMB, J. D. (1981). *Acta Cryst.* **B37**, 1664–1669.

CAMPBELL, M. L., LARSON, S. B. & DALLEY, N. K. (1981*a*). *Acta Cryst.* **B37**, 1741–1744.

CAMPBELL, M. L., LARSON, S. B. & DALLEY, N. K. (1981*b*). *Acta Cryst.* **B37**, 1744–1747.

CHACKO, K. K., RUBAN, G. A., AOKI, K. & WEBER, E. (1988). *Acta Cryst.* **C44**, 352–355.

CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891-1898.

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* **A24**, 321–324.

DALLEY, N. K. (1978). *Synthetic Multidentate Macrocyclic Compounds*, edited by R. M. IZATT & J. J. CHRISTENSEN, Ch. 4, *Structual Studies*, pp. 207–243. New York: Academic Press.

DUNITZ, J. D., DOBLER, M., SEILER, P. & PHIZACKERLEY, R. P. (1974). *Acta Cryst.* **B30**, 2733–2738.

FRENSDORFF, H. K. (1971). *J. Am. Chem. Soc.* **93**, 600–606.

GIBBONS, C. S. & TROTTER, J. (1971). *J. Chem. Soc. A*, pp. 2058–2062.

GOLDBERG, I. (1975). *Acta Cryst.* **B31**, 754–762.

HILGENFELD, R. & SAENGER, W. (1982). *Top. Curr. Chem.* **101**, 1–84.

IZATT, R. M., TERRY, R. E., HANSEN, L. D., AVONDET, A. G., BRADSHAW, J. S., DALLEY, N. K., JENSEN, T. E., CHRISTENSEN, J. J. & HAYMORE, B. L. (1978). *Inorg. Chim. Acta*, **30**, 1–8.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

LOUIS, P. R., AGNUS, Y. & WEISS, R. (1977). *Acta Cryst.* **B33**, 1418–1421.

LOUIS, P. R., PELISSARD, D. & WEISS, R. (1976). *Acta Cryst.* **B32**, 1480–1485.

MERCER, M. & TRUTER, M. R. (1973) *J. Chem. Soc. Dalton Trans.* pp. 2215–2220.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

NORTH, A. C. T., PHILLIPS, D. C. & MATHEWS, F. S. (1968). *Acta Cryst.* **A24**, 351–359.

PAULING, L. (1960). *The Nature of the Chemical Bond*, 3rd ed., p. 260. Ithaca: Cornell Univ. Press.

SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

STEWART, R.F. , DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

TAYLOR, R. & KENNARD, O. (1982). *J. Am. Chem. Soc.* **104**, 5063–5070.

WEBER, E. & VOGTLE, F. (1976). *Justus Liebigs Ann. Chem.* pp. 891-915.

WEBER, G. (1982). *Inorg. Chim. Acta*, **58**, 27–33.

WEBER, G., JONES, P. G. & SHELDRICK, G. M. (1983). *Acta Cryst.* **C39**, 389–391.

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Structure of Inosinium Tetrabromoaurate(III) Dihydrate

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Abstract. Inosinium tetrabromoaurate(III) dihydrate, $C_{10}H_{13}N_4O_5^+.[AuBr_4]^-.2H_2O$, $M_r = 821{\cdot}85$, triclinic, $P1$, $a = 7{\cdot}430$ (1), $b = 8{\cdot}272$ (2), $c = 8{\cdot}768$ (3) Å, $\alpha = 98{\cdot}96$ (2), $\beta = 108{\cdot}02$ (2), $\gamma = 94{\cdot}56$ (2)°, $V = 501{\cdot}50$ Å^3, $Z = 1$, $D_x = 2{\cdot}721$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 23{\cdot}82$ mm^{-1}, $F(000) = 380$, $T = 296$ K, final $R = 0{\cdot}045$ for 1790 unique observed reflections. The unit cell contains square-planar $AuBr_4^-$ anions and N(7)-protonated inosine units.

Introduction. Interest in gold coordination chemistry has been growing in recent years as a consequence of

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