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Sodium tetrabromoaurate(III) dihydrate

Richard Welter,[a]* Hedi Omrani[b] and Rene Vangelisti[c]

[a]Laboratoire de Chimie des métaux de transition (UMR 7513 CNRS), Université Louis Pasteur, 4 rue Blaise Pascal, F-67070 Strasbourg CEDEX, France, [b]Faculté des Sciences, Département de Chimie, Monastir 5000, Tunisia, and [c]Labor-Minéral, UMR 7555, Université Henri Poincaré Nancy I, Faculté des Sciences, BP 239, 54506 Vandoeuvre les Nancy CEDEX, France

Correspondence e-mail: welter@chimie.u-strasbg.fr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Au–Br) = 0.002 Å
R factor = 0.049
wR factor = 0.097
Data-to-parameter ratio = 25.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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The structure of the title compound, $NaAuBr_4{\cdot}2H_2O$ is isomorphous with that of $NaAuCl_4{\cdot}2H_2O$. The Na, Au and Br atoms lie on the mirror plane. The $AuBr_4^-$ anions are nearly square planar with Au—Br bond lengths in the range 2.415 (2)–2.433 (2) Å.

Comment

Previous studies concerning the crystal structure determination of the anhydrous $MAuX_4$ compounds and the corresponding dihydrate $MAuX_4{\cdot}2H_2O$ (M is Na or K, X is Cl or Br) have shown that: (i) $KAuBr_4$ (Omrani *et al.*, 1999), $KAuBr_4{\cdot}2H_2O$ (Omrani *et al.*, 1986), $KAuCl_4$ (Jones & Bembenek, 1992) and $NaAuCl_4$ (Jones *et al.*, 1988) crystallize in the monoclinic system with the space group $P2_1/c$ (or $P2_1/n$); (ii) $NaAuCl_4{\cdot}2H_2O$ (Bonamico & Dessy, 1965) and $KAuCl_4{\cdot}2H_2O$ (Theobald & Omrani, 1980) crystallize in the orthorhombic system with the space group *Pnma* and *Pbcn*, respectively. All these compounds are characterized by the occurrence of square-planar AuX_4^- anions with typical Au—X distances (approximately 2.29 Å for Au—Cl bond and 2.43 Å for Au—Br bond). In this class of based gold coordination compounds, only both $NaAuBr_4$ and $NaAuBr_4{\cdot}2H_2O$ compounds were not yet characterized. In the present work, we report on the crystal structure of the dihydrate.

The structure of the title compound, $NaAuBr_4{\cdot}2H_2O$, (I), is isomorphous with that of $NaAuCl_4{\cdot}2H_2O$ (Bonamico & Dessy, 1965). The orthorhombic cell contains four Au atoms and the $AuBr_4^-$ anions are nearly square planar (Fig. 1). The Au, Br and Na atoms lie on the mirror plane. The structure can also be described as a pseudo-lamellar compound in which the $NaAuBr_4$ planes (at $y = \frac{1}{4}$ and $\frac{3}{4}$) are piled up along the b axis and connected *via* Na—O—Na bonds. There is only one independent Na atom, which is coordinated by four O atoms at distances in the range 2.437 (12)–2.509 (13) Å and three Br atoms at distances in the range 3.150 (10)–3.300 (10) Å (Table 1).

Experimental

Crystals were prepared by dissolving powder of $NaAuCl_4{\cdot}2H_2O$ in aqueous HBr (1 M). The solution was slowly evaporated (two months) at 300 K. After complete crystallization, dark brick red crystals were obtained. A single-crystal was then sealed in Lindemann glass capillary.

Crystal data

$NaAuBr_4 \cdot 2H_2O$
$M_r = 575.63$
Orthorhombic, *Pnma*
$a = 13.320\ (6)$ Å
$b = 7.253\ (2)$ Å
$c = 9.420\ (3)$ Å
$V = 910.1\ (6)$ Å^3
$Z = 4$
$D_x = 4.201$ Mg m^{-3}
Ag $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 8.3$–$10.4°$
$\mu = 18.20$ mm^{-1}
$T = 293\ (2)$ K
Parallelepiped, dark red
$0.16 \times 0.09 \times 0.06$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (*SORTAV*; Blessing, 1987)
$T_{min} = 0.051$, $T_{max} = 0.363$
1368 measured reflections
1368 independent reflections
905 reflections with $I > 2\sigma(I)$
$\theta_{max} = 22.9°$
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 13$
2 standard reflections
frequency: 180 min
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.097$
$S = 1.09$
1368 reflections
54 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2 + 12.7490P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.09$ e Å^{-3}
$\Delta\rho_{min} = -1.57$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0047 (3)

Table 1
Selected geometric parameters (Å, °).

Au—Br4	2.415 (2)	Br4—Na	3.300 (10)
Au—Br3	2.427 (2)	Na—O	2.437 (12)
Au—Br1	2.431 (2)	Na—O^{ii}	2.437 (12)
Au—Br2	2.433 (2)	Na—O^{iii}	2.509 (13)
Br1—Na^{i}	3.163 (9)	Na—O^{iv}	2.509 (13)
Br3—Na^{i}	3.150 (10)		
Br4—Au—Br3	88.41 (8)	Br4—Au—Br2	90.19 (8)
Br4—Au—Br1	180.00 (8)	Br3—Au—Br2	178.60 (7)
Br3—Au—Br1	91.59 (8)	Br1—Au—Br2	89.81 (8)

Symmetry codes: (i) $x, y, z-1$; (ii) $x, \frac{1}{2}-y, z$; (iii) $1-x, \frac{1}{2}+y, 1-z$; (iv) $1-x, -y, 1-z$.

In the final electron-density difference map, both minimum (−1.57 e Å^{-3} at 0.3594,0.2500,0.5494) and maximum (2.09 e Å^{-3} at 0.4964,0.1831,0.2760) occur respectively at 0.96 Å away from Br4 and 1.72 Å from Na. They may be due to the irregular crystal shape and the approximate absorption correction. The H atoms were fixed with O—H distances of 0.95 Å.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CADAK* and *SORTAV* (Blessing, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 1995); software used to prepare material for publication: *SHELXL*97.

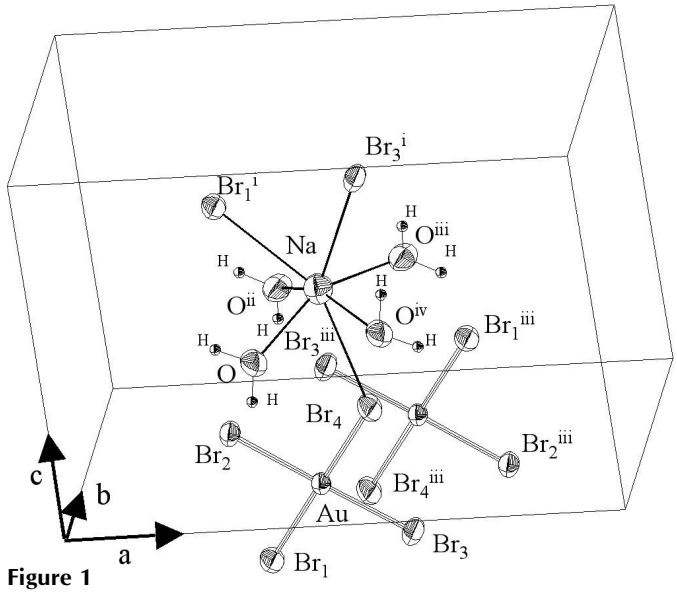

Figure 1
Part of the crystal structure. Displacement ellipsoids are shown at 50% probability levels. Symmetry codes: (i) $x, y, z-1$; (ii) $x, \frac{1}{2}-y, z$; (iii) $1-x, \frac{1}{2}+y, 1-z$; (iv) $1-x, -y, 1-z$.

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