Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetraaqua(nitromethane)potassium bromide monohydrate

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Received 14 November 2000
Accepted 20 December 2000
Online 10 January 2001

Each K^+ ion in $[K(CH_3NO_2)(H_2O)_4]Br\cdot H_2O$, (I), has an eightfold coordination, with the coordination sphere containing four water molecules and four O atoms from the nitromethane molecules. The coordination polyhedra share two O atoms from two different nitromethane molecules and, in this way, form chains running parallel to the (100) direction. Hydrogen bonding involving the Br^- ion and the fifth water molecule tie the chains together.

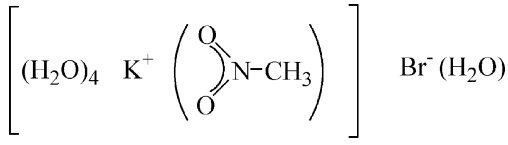
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.008 Å
R factor = 0.037
wR factor = 0.092
Data-to-parameter ratio = 9.5

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

Experimental

The title material, (I), was found as a side product in the attempted preparation of the linear chain compound Cu(14ane)$CuBr_4$ (where 14ane is 1,4,8,11-tetraazacyclotetradecane), similar to the corresponding chloride material (Wang *et al.*, 1996). The process involved slow crystallization of a solution of $CuBr_2$ and 14ane in an organic solvent contained in a sealed vial. The major product obtained was the mixed valence compound Cu(14ane)$CuBr_3$ (Willett, 2001). Further examination of the solid material obtained revealed a few small colorless crystals. With the possibility that this was a further product containing only the Cu^I metal ion, a crystal was selected for single-crystal structure determination.



(I)

Crystal data

$[K(CH_3NO_2)(H_2O)_4]Br\cdot H_2O$
M_r = 270.13
Monoclinic, $P2_1/n$
a = 6.8004 (3) Å
b = 13.8358 (5) Å
c = 10.8658 (4) Å
β = 97.896 (1)°
V = 1012.66 (7) Å^3
Z = 4
D_x = 1.772 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4394 reflections
θ = 2.4–23.3°
μ = 4.47 mm^{-1}
T = 293 (2) K
Needle, colorless
0.50 × 0.05 × 0.05 mm

Data collection

SMART 1000 area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*XPREP* in *SHELXTL*; Sheldrick, 1997*b*)
T_{min} = 0.718, T_{max} = 0.800
4394 measured reflections
1446 independent reflections
1362 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 23.3°
$h = -7 \rightarrow 7$
$k = -15 \rightarrow 15$
$l = -11 \rightarrow 12$
50 standard reflections
frequency: beginning and end of collection
intensity decay: 2.6%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 2.7724P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.092$	$\Delta\rho_{max} = 0.44$ e Å^{-3}
$S = 1.10$	$\Delta\rho_{min} = -0.52$ e Å^{-3}
1446 reflections	Extinction correction: *SHELXL*97
153 parameters	Extinction coefficient: 0.0036 (14)
All H-atom parameters refined	

H atoms were located *via* difference syntheses and their positions were loosely constrained to expected geometry *via* the *DFIX* instruction in *SHELXL*97. Their isotropic displacement parameters were not constrained.

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL*97.

The use of the Single Crystal Diffraction Facility of the University Research Office at the University of Idaho is greatly appreciated.

References

Bruker (1996). *SMART* (Version 4.045) and *SAINT* (Version 4.035). Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

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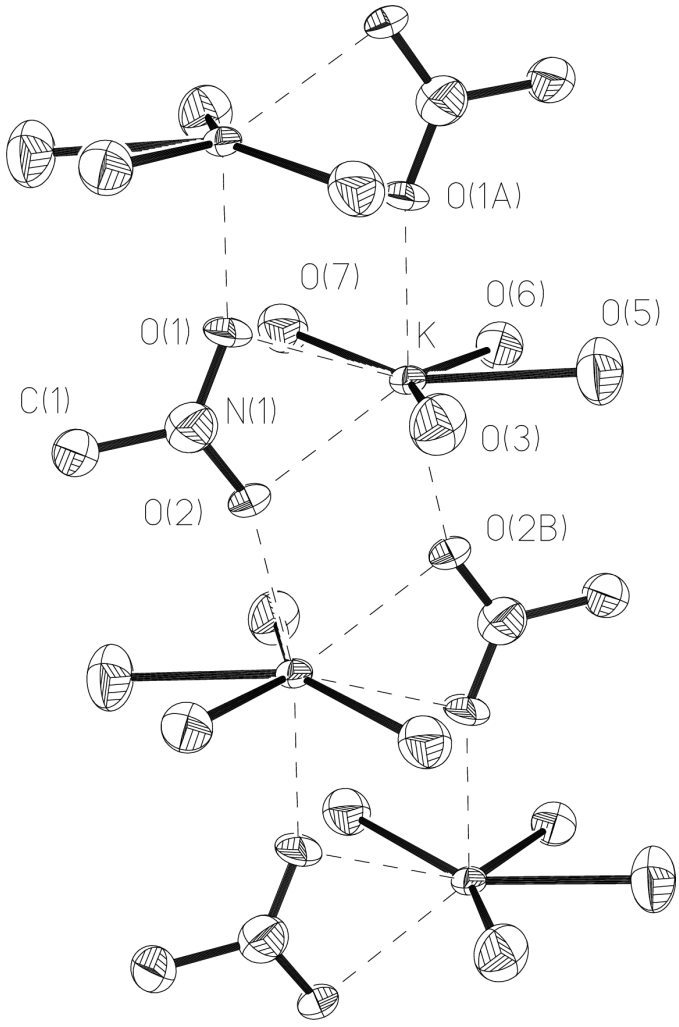

Figure 1
Illustration of the chain structure of the title compound. Displacement ellipsoids are shown at the 50% probability level.