Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ammonium mercury(II) dichloride nitrate, $(NH_4)_2HgCl_2(NO_3)_2$

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Received 17 June 2002
Accepted 21 June 2002
Online 12 July 2002

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Hg–Cl) = 0.001 Å
H-atom completeness 0%
R factor = 0.019
wR factor = 0.047
Data-to-parameter ratio = 15.7

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

The title compound, $(NH_4)_2HgCl_2(NO_3)_2$, is a double salt of $HgCl_2$ and NH_4NO_3 and can also be written as '$HgCl_2{\cdot}2NH_4NO_3$'. The structure contains $HgCl_2$ units which are connected by nitrate groups, through long links of *ca.* 2.90 Å, to give chains running along [010]. All atoms apart from the two oxygen atoms are located on a mirror plane perpendicular to the *b* axis. The coordination around mercury is a distorted hexagonal bipyramid.

Comment

Structures containing both the nitrate and chloride anions are quite rare, as can be seen from a search in the ICSD database. One example is the structure of $CaCl(NO_3){\cdot}2H_2O$ reported by Leclaire & Borel (1978). Carter & Zompa (1999) reported the structure of a double anion salt, $(NH_4)_3[ZnCl_4]NO_3$, containing tetrahedral $ZnCl_4^{2-}$ and NO_3^- anions. The structure of the title compound, $(NH_4)_2HgCl_2(NO_3)_2$, consists of $HgCl_2$ units which are almost parallel to [001]. They are connected into rows parallel to [010] by weak interactions to two types of nitrate groups. One nitrate group, around N1 (parallel to the *ab* plane), bridges two $HgCl_2$ units with the distances Hg1···O1 = 2.790 (1) Å and Hg1···O2 = 2.865 (3) Å. The second nitrate group, around N2 (parallel to the *ac* plane), bridges two $HgCl_2$ units with a long distance of Hg1···O3 = 2.968 (3) Å. These links complete the effective coordination sphere of mercury to a '2+6' hexagonal bipyramid. The distances Hg1···Cl1 and Hg1···Cl2 of about 2.30 Å are in the usual range.

Experimental

A solution of 20 mmol (0.1608 g) NH_4NO_3 and 10 mmol (0.2715 g) $HgCl_2$ in a mixture of 20 ml water and 20 ml methanol was stirred at 333 K for 3 h. Single crystals of the title compound were obtained after leaving the solution at room temperature for 3 d.

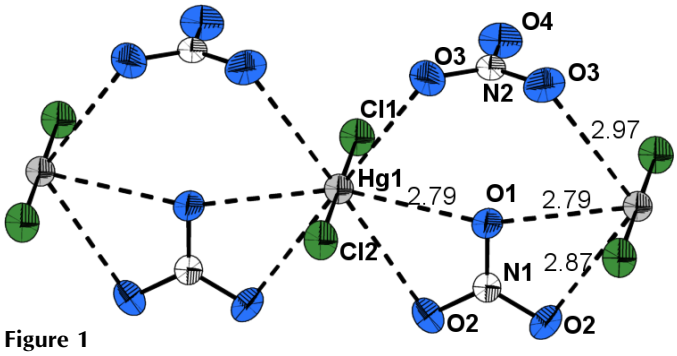

Figure 1
$HgCl_2$ units connected by nitrate groups to rows along [010] in $(NH_4)_2HgCl_2(NO_3)_2$, with labelling and displacement ellipsoids drawn at the 50% probability level.

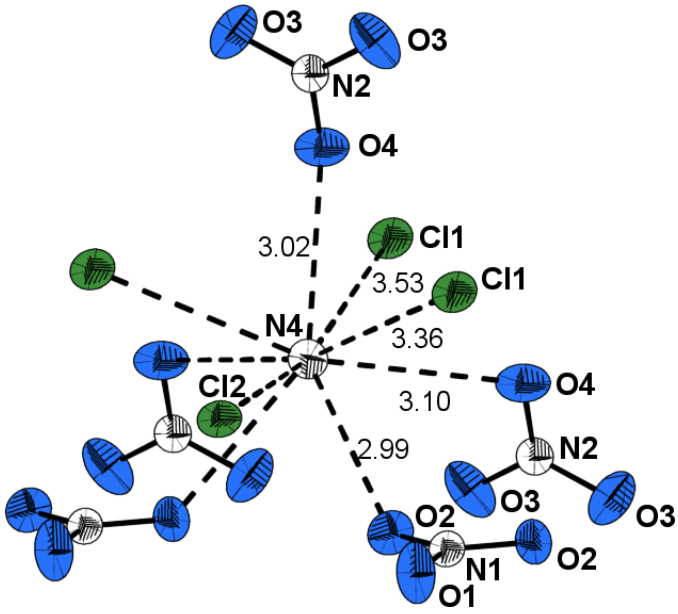

Figure 2
The environment of the ammonium ions in $(NH_4)_2HgCl_2(NO_3)_2$.

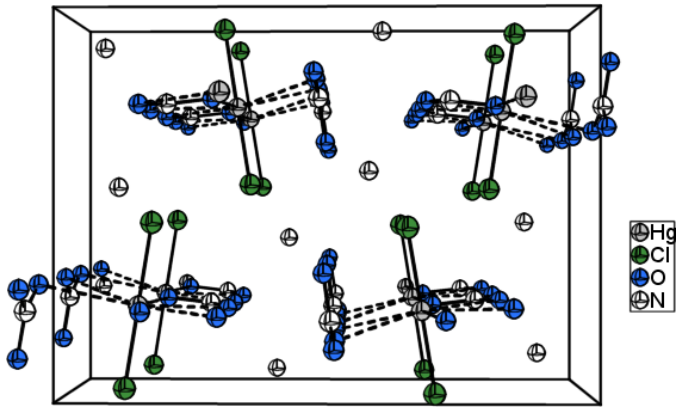

Figure 3
View of the unit cell contents along [010].

Table 1
Selected geometric parameters (Å, °).

Hg1—Cl1	2.3007 (13)	O2—N1	1.245 (4)
Hg1—Cl2	2.3082 (13)	O3—N2	1.243 (3)
O1—N1	1.249 (6)	O4—N2	1.227 (5)
Cl1—Hg1—Cl2	179.75 (5)	O4—N2—O3^{i}	120.1 (2)
O2^{i}—N1—O2	120.8 (5)	O3^{i}—N2—O3	119.7 (5)
O2^{i}—N1—O1	119.6 (2)		

Symmetry code: (i) $x, \frac{1}{2}-y, z$.

Crystal data

$(NH_4)_2HgCl_2(NO_3)_2$	Mo $K\alpha$ radiation
M_r = 431.59	Cell parameters from 23769 reflections
Orthorhombic, *Pnma*	θ = 2.2–27.0°
a = 15.5758 (16) Å	μ = 16.49 mm^{-1}
b = 5.4976 (5) Å	T = 293 (2) K
c = 11.2826 (15) Å	Prism, colourless
V = 966.12 (18) Å^3	0.3 × 0.2 × 0.1 mm
Z = 4	
D_x = 2.967 Mg m^{-3}	

Data collection

Stoe Imaging Plate Diffraction System diffractometer	1163 independent reflections
φ scans	983 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)	R_{int} = 0.061
T_{min} = 0.027, T_{max} = 0.192	θ_{max} = 27.0°
14614 measured reflections	$h = -19 \rightarrow 19$
	$k = -7 \rightarrow 6$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.019	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.047	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
S = 0.94	$\Delta\rho_{min}$ = −0.67 e Å^{-3}
1163 reflections	Extinction correction: *SHELXL*97
74 parameters	Extinction coefficient: 0.0053 (2)
H atoms not located	

H atoms were not located and were not included in the refinement

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-STEP*32 (Stoe & Cie, 2000); data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL*97.

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