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Holmium chloride oxoselenate(IV), $HoClSeO_3$

Mathias S. Wickleder

Institut für Anorganische Chemie, Universität zu Köln, Greinstr. 6, D-50939 Köln, Germany

Correspondence e-mail: mathias.wickleder@uni-koeln.de

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Se–O) = 0.004 Å
R factor = 0.023
wR factor = 0.053
Data-to-parameter ratio = 19.7

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

In the title compound, $HoClSeO_3$, the Ho^{3+} ion is coordinated by three monodentate SeO_3^{2-} ions, one chelating selenite group, and two chloride ligands. The $[HoO_5Cl_2]$ polyhedra are pentagonal bipyramids which are connected to form a three-dimensional network *via* edges and vertices. The SeO_3^{2-} ion shows the typical pyramidal shape due to the lone electron pair of the selenium atom.

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Comment

$HoClSeO_3$ is isotypic with the recently described $ErClSeO_3$ (Wickleder, 2002) and also with the chloride tellurite $HoClTeO_3$ (Meier & Schleid, 2002). Isotypism of rare earth selenites and tellurites is very rare, due to the tendency of Te^{4+} to attain higher coordination numbers. In the crystal structure of $HoClSeO_3$, the Ho^{3+} ion is coordinated by five O atoms, with Ho—O distances ranging from 2.201 (5) to 2.373 (4) Å, and two chloride ligands at 2.7033 (17) and 2.7264 (18) Å. The $[HoO_5Cl_2]$ polyhedron is best regarded as a pentagonal bipyramid, with an O atom and a chloride ion at the apices. The linkage of the polyhedra occurs in the [010] direction *via* opposite O1—O1 edges, leading to infinite chains (Fig. 1), which are further connected *via* chloride ions into a three-dimensional network. The O atoms within the $[HoO_5Cl_2]$ polyhedra belong to three monodentate and one chelating SeO_3^{2-} ions. The monodentate ions are chelating and the chelating ones are monodentate to the adjacent polyhedra. The chloride ion is twofold coordinated and the SeO_3^{2-} group is connected to four Ho^{3+} ions. When viewed along [010], the effect of the stereochemically active lone electron pairs at the Se atoms is obvious (Fig. 2).

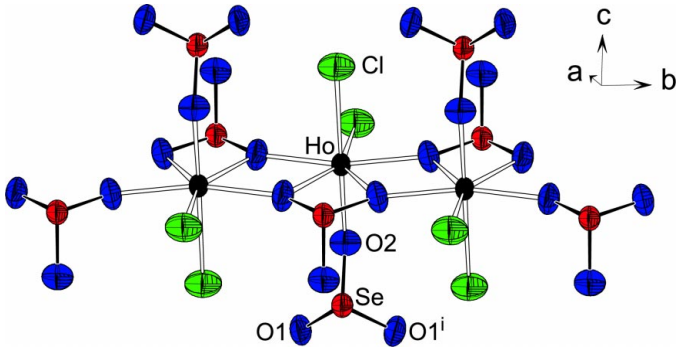

Figure 1
Linkage of the $[HoO_5Cl_2]$ polyhedra into chains in the crystal structure of $HoClSeO_3$. Note that one selenite group acts as a chelating ligand. Displacement ellipsoids are drawn at the 90% probability level. [Symmetry code: (vi) $x, -y+\frac{1}{2}, z$]

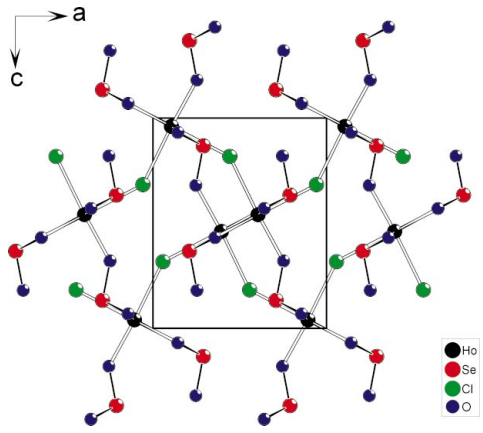

Figure 2
Projection of the crystal structure of $HoClSeO_3$ on (010).

Experimental

A mixture of Ho_2O_3, $HoCl_3$, and SeO_2 (molar ratio 1:1:3) was heated in an evacuated silica ampoule to 573 K with the help of a resistance furnace. After 24 h the temperature was raised to 1023 K, followed by slow cooling (5 K h^{-1}) to 303 K. The light yellow, slightly moisture-sensitive crystals were handled in an argon-filled glove box and an appropriate specimen was mounted in a glass capillary for the X-ray investigation.

Crystal data

$ClHoO_3Se$
M_r = 327.34
Orthorhombic, *Pnma*
a = 7.2093 (15) Å
b = 6.9259 (10) Å
c = 8.7689 (15) Å
V = 437.84 (13) Å^3
Z = 4
D_x = 4.966 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2000 reflections
θ = 3.0–28.0°
μ = 26.85 mm^{-1}
T = 293 (2) K
Column, yellow
0.15 × 0.13 × 0.12 mm

Data collection

Stoe IPDS-I diffractometer
φ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1999)
T_{min} = 0.023, T_{max} = 0.039
4891 measured reflections
688 independent reflections
626 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 30.0°
$h = -10 \rightarrow 10$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.053
S = 1.04
688 reflections
35 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.21 e Å^{-3}
$\Delta\rho_{min}$ = −1.79 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0412 (15)

Table 1
Selected geometric parameters (Å, °).

Ho—O2^{i}	2.201 (5)	Ho—Cl^{i}	2.7033 (17)
Ho—O1^{ii}	2.266 (3)	Ho—Cl	2.7264 (18)
Ho—O1^{iii}	2.266 (3)	Se—O2	1.664 (5)
Ho—O1^{iv}	2.373 (4)	Se—O1^{vi}	1.718 (3)
Ho—O1^{v}	2.373 (4)	Se—O1	1.718 (3)
O2—Se—O1^{vi}	102.11 (19)	O1^{vi}—Se—O1	91.1 (2)
O2—Se—O1	102.11 (18)		

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

The maximum and minimum residual electron-density peaks are 1.14 and 0.85 Å from the Ho atom.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL*97 (Sheldrick, 1997).

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