Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Strontium chlorite, $Sr(ClO_2)_2$, from X-ray powder diffraction data

Anton I. Smolentsev* and Dmitry Yu. Naumov

Nikolaev Institute of Inorganic Chemistry, SB Russian Academy of Sciences, Akad. Lavrentiev prosp. 3, Novosibirsk 90, 630090, Russian Federation

Correspondence e-mail: smolentsev@ngs.ru

Key indicators

Powder X-ray study
T = 293 K
Mean σ(Cl–O) = 0.006 Å
R factor = 0.136
wR factor = 0.165
Data-to-parameter ratio = 8.21

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

Received 7 October 2005
Accepted 21 October 2005
Online 27 October 2005

The structure of strontium chlorite, $Sr(ClO_2)_2$, has been refined from X-ray powder diffraction data using the Rietveld method. The compound crystallizes in the orthorhombic space group *Ccca* (*Ccce*), with Z = 4. The structure is based on separate layers parallel to the *ac* plane, consisting of strontium cations that are coordinated by chlorite anions; the O atoms form almost ideal square antiprisms. Within the layers, each anion bridges four metal cations. The Sr atoms are located on special positions of 222 symmetry, the Cl atoms lie on twofold axes and the O atoms are in general positions. The compound is isostructural with calcium chlorite, $Ca(ClO_2)_2$, and lead chlorite, $Pb(ClO_2)_2$.

Comment

The present paper reports the results of an X-ray powder diffraction study of strontium chlorite. It continues our systematic structural investigation of alkaline earth metal chlorites, which includes $Ca(ClO_2)_2$ (Smolentsev & Naumov, 2005). The title compound is isostructural with the calcium salt and also with $Pb(ClO_2)_2$ (Okuda *et al.*, 1990), whose structure was used as a trial structure for the Rietveld refinement. As a representation of the refinement results, the experimental and calculated powder profiles and the difference between them are shown in Fig. 1. For the general structure discussion, see Smolentsev & Naumov (2005). Compared with the calcium compound, in $Sr(ClO_2)_2$, different M—O distances [2.615 (6) and 2.657 (6) Å in $Sr(ClO_2)_2$ *versus* 2.481 (3) and 2.499 (3) Å in $Ca(ClO_2)_2$] are realized, while the Cl—O distances and O—

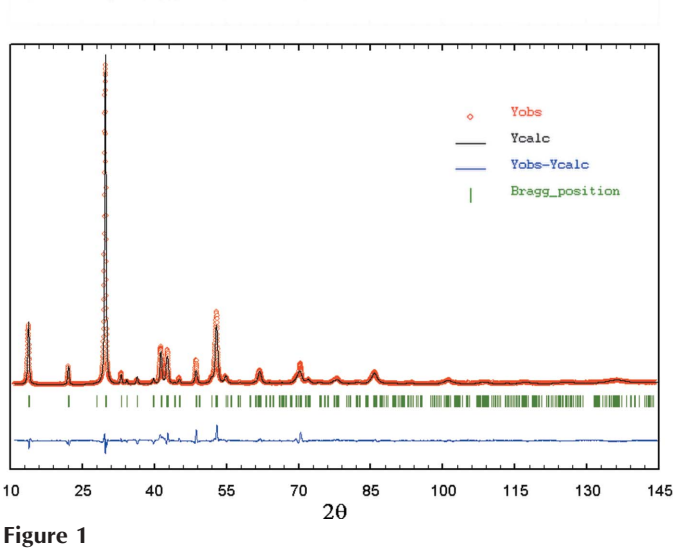

Figure 1
Experimental and calculated powder profiles of $Sr(ClO_2)_2$, with difference plot.

Cl—O angles in the chlorite anion are very similar [1.570 (6) Å and 110.6 (6)° *versus* 1.585 (3) Å and 115.3 (3)°].

Experimental

Polycrystalline $Sr(ClO_2)_2$ was synthesized at room temperature by reacting an aqueous suspension of strontium peroxide with an excess of chlorine dioxide, followed by precipitation from solution by adding a 3:1 mixture of ethanol and diethyl ether. A white crystalline powder resulted.

Crystal data

$Sr(ClO_2)_2$
M_r = 222.52
Orthorhombic, *Ccca* (*Ccce*)
a = 5.9799 (12) Å
b = 12.7519 (16) Å
c = 5.9787 (12) Å
V = 455.92 (11) Å^3
Z = 4
D_x = 3.242 Mg m^{-3}
Cu $K\alpha$ radiation
Wavelength of incident radiation: 1.54178 Å
T = 293 (2) K
Specimen shape: flat sheet
10 × 10 × 0.1 mm
Particle morphology: plate-like, white

Data collection

Philips PW1700 powder diffractometer
Specimen mounting: drifted powder on standard quartz sample holder
Specimen mounted in reflection mode
Scan method: step
$2\theta_{min}$ = 5.0, $2\theta_{max}$ = 145.0°
Increment in 2θ = 0.02°

Refinement

R_p = 0.136
R_{wp} = 0.165
R_{exp} = 0.055
R_B = 0.057
S = 3.03
Profile function: split pseudo-Voigt
230 reflections
28 parameters
$w = 1/[\sigma^2(Y_i)]$
$(\Delta/\sigma)_{max}$ = 0.01
Preferred orientation correction: $I_{corr} = I_{obs}[G_2 + (1 - G_2) \times \exp(G_1\alpha^2)]$, where α is the acute angle between the scattering vector and the normal to the crystallites, G_1 = −0.54 (5), G_2 = 0.29 (3), axis [010] (Rietveld, 1969)

Table 1
Selected geometric parameters (Å, °).

Sr—O	2.615 (6)	Cl—O	1.570 (6)
Sr—O^{i}	2.657 (6)		
O—Cl—O^{ii}	110.6 (6)		

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

The powder pattern indexing and Rietveld refinement of the structure model were performed as described by Smolentsev & Naumov (2005).

Data collection: *APD1700 Software* (Philips, 1989); cell refinement: *FULLPROF2k* (Rodriguez-Carvajal, 2004); program(s) used to refine structure: *FULLPROF2k*; graphics: *WINPLOTR* (Roisnel & Rodriguez-Carvajal, 2005); software used to prepare material for publication: *WINPLOTR*.

The authors thank N. V. Kuratieva for useful comments during the preparation of this paper.

References

Okuda, M., Ishihara, M., Yamanaka, M., Ohba, S. & Saito, Y. (1990). *Acta Cryst.* C**46**, 1755–1759.
Philips (1989). *APD1700 Software*. Version 4.0. Philips Electronics Inc., Natick, MA, USA.
Rietveld, H. M. (1969). *J. Appl. Cryst.* **2**, 65–71.
Rodriguez-Carvajal, J. (2004). *FULLPROF2k*. Version of November 2004. Laboratoire Leon Brillouin (CEA/CNRS), CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France.
Roisnel, T. & Rodriguez-Carvajal, J. (2005). *WINPLOTR*. Version of February 2005. Laboratoire Leon Brillouin (CEA/CNRS), CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France.
Smolentsev, A. I. & Naumov, D. Y. (2005). *Acta Cryst.* E**61**, i246–i248.