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Case Report

Refined Crystal Structure of Scandium Oxide-Hydroxide, α- ScO(OH)

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Abstract

Background: Fundamental chemical compounds are often insufficiently studied or require structural refinement. This applies in particular to halides, sulfides or oxide's structure types, which are the basis for crystal chemical studies and synthesis of inorganic compounds.

Case: We report a structure refinement of ScO(OH) oxide-hydroxide previously investigated at an insufficient level. A search for additional electron density allowed localization of H atom position via electron density maxima and its refinement. A strong hydrogen bond is fixed. Comparison with the mineral diaspore demonstrated similarity of the synthetic and natural compounds.

Conclusion: The results highlight the importance of high-precision X-ray diffraction analysis for determining structural parameters, hydrogen atom localization, and chemical bonds in the structure.

Keywords: Sc oxide-hydroxide; Single crystal synthesis; X-ray diffraction and Structure refinement; Hydrogen bonds; Minerals analogue

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Introduction

Inorganic compounds with Rare Earth Elements (REE) attract attention in the last time because of many properties as laser, Nonlinear Optical (NLO) or luminescent materials. However up to now simplest compounds with REE are not sufficiently investigated. One example of such a case is scandium oxide-hydroxide α-ScO(OH) whose structure was solved only in 1967 [1] with a sufficient high R=8.5%.

Scandium oxide-hydroxide was synthesized repeatedly under hydrothermal conditions. For this purpose, $Sc(NO_3)_2 \cdot 4H_2O$ (1g, 3.3mmol) were dissolved in 3mL of distilled water and mixed with 2ml. of a 40% NaOH solution, with constant stirring. The resulting suspension was transferred to a 7mL stainless steel autoclave. The autoclaves were closed and placed in a furnace, where they were heated to 554K for 24h and kept at this temperature for 7 days. After the reaction, the autoclave was allowed to cool naturally for 10h. The precipitate was separated by filtration, washed with hot distilled water, dried at room temperature. The mass yield of the experiment was 100%. Resynthesized crystals were transparent, colorless and light-honey, isometric, rectangular and possessed high quality. That stimulated to carry out the refinement of this basal compound with Sc.

Case Description

A colorless rectangular crystal, size 0.063×0.093×0.128mm was select for X-ray diffraction experiment carried out on X calibur S, w-scaning, Mo Kα-radiation (0.71073Å). It was registered 1170 reflections averaged to 229 used in the refinement with Iobs >2 sigma (Iobs).

The refinement was carried out in *Pnam* sp.group (*Pnma* standard) using the initial atomic coordinates from [1]. The asymmetric unit of α-ScO(OH) contains three unique atoms on special positions on mirror plane: one Sc atom and two oxygen atoms. Residual electron density gave maxima on distance 0.75Å from O2 which was added in the model as H-atom.

Bond-valence sums calculations [2] confirmed O(2) as hydroxyl position with the sum 1.40 compared to 1.74 on O(1); Sc has 3.14. Isotropic approximation of atoms displacements parameters gave R=0.0297 and allowed to apply anisotropic displacements with decrease in R up to 0.0275. The distance from donor DO (2) to H was changed up to 0.55Å with the distance to acceptor A O(1) H… A=1.81Å. The proton position was determined on the base of known distance of 0.99Å H-O and its coordinates were calculated. The angles D-Helectron..A is 169,7°, the angle D-Hproton..A is 165° in the hydrogen bond D-A=2.785Å. The obtained geometrical characteristics give evidence that it is strong hydrogen bond.

Discussion

The α-ScO(OH) structure is constructed from octahedra joined by edges in bands along c-axis (Figure 1, left and right) with chessboard order fixed in the ab projection. Hydrogen bonds are directed via channels from one band to another connecting them. The structure possesses hexagonal close-packing visible well in Figure, right. Rutile-like chains may be selected. The α-ScO(OH) structure is identical to well-studied α-AlO (OH) diaspore mineral [3] despite the different unit cell setting, and the hydrogen bonds are also equal. The third member of family is α-FeO(OH) goethite mineral [3]. All three Al-, Fe-, Sc-oxide- hydroxide have except α-modifications, also equal each other γ-modifications with the sp. group *Cmcm* and coordination polyhedra not octahedra, but trigonal pyramid with one split corner. The projection of framework structure is shown in the Figure on the left, a band of octahedra is shown on the right. All the atoms occupy 4c Wyckoff positions of the space group and the refined coordinates are given under the figures. The compound is deposited in CCDC no. 2479689 [4,5].

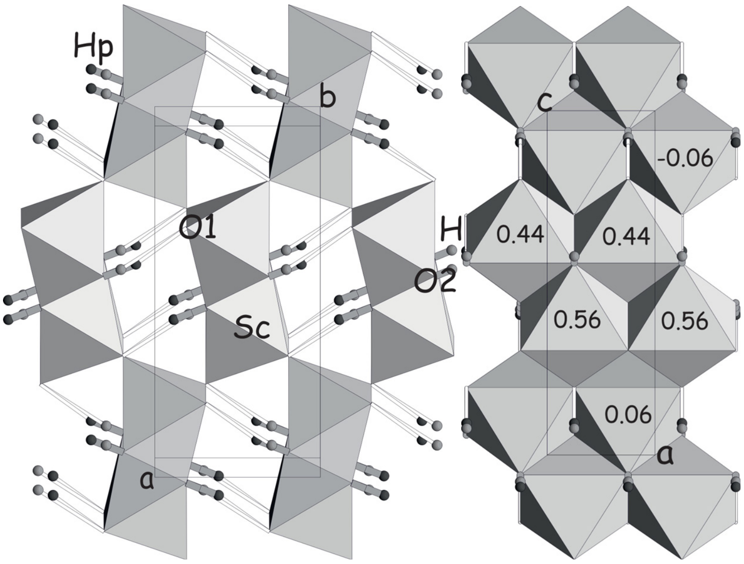

Figure 1:
Sc -0.14507(6) 0.06472(1) 0.25
O(1) 0.19611(3) 0.6920(5) 0.25
O(2) 0.05751(3) 0.19093(7) 0.25
H .0773(5) 0.2944(10) 0.25

Conclusion

ScO(OH) with the smallest REE element Sc was re-synthesized and single crystals of good quality were obtained. The refinement improved R-factor from 0.085 to 0.0297 allowing us to determine the hydrogen atom position based on their electron density and approximate the proton position. Analogues with minerals are provided.

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