

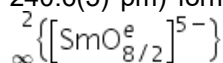
**MS15-1-4 SmBi<sub>2</sub>O<sub>4</sub>Cl: the first single-crystal study in the systems LnBi<sub>2</sub>O<sub>4</sub>X**  
**#MS15-1-4**

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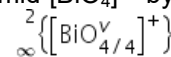
**Abstract**

A mixture of Bi<sub>2</sub>O<sub>3</sub>, Sm<sub>2</sub>O<sub>3</sub> and SmCl<sub>3</sub> reacted at 800 °C in an eutectic mixture of NaCl and CsCl as flux in a fused silica ampoule and resulted in yellow plates of the title compound. SmBi<sub>2</sub>O<sub>4</sub>Cl crystallizes in the tetragonal space group *P4/mmm* with the lattice parameters *a* = 388.91(3) pm and *c* = 895.16(7) pm with *Z* = 4 and hitherto its structure was only known from X-ray powder diffraction data [1]. The corresponding antimonate(III) SmSb<sub>2</sub>O<sub>4</sub>Cl with the real composition Sm<sub>1.3</sub>Sb<sub>1.7</sub>O<sub>4</sub>Cl offers a mixed occupation of the antimony position with samarium [2,3] for the same crystal structure. In contrast to this, SmBi<sub>2</sub>O<sub>4</sub>Cl shows no mixed occupation, but one samarium and one bismuth position with regular occupation.

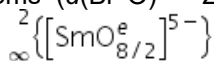
The structure features one crystallographic samarium (1*a*: 0, 0, 0), one bismuth (2*h*: 1/2, 1/2, 0.28294(9)), one oxygen (4*i*: 0, 1/2, 0.1582(9)) and one chlorine position (1*b*: 0, 0, 1/2) each. Sm<sup>3+</sup> is coordinated by eight oxygen atoms (*d*(Sm–O) = 240.6(5) pm) forming a [SmO<sub>8</sub>]<sup>13-</sup> cube. Each cube is connected via edges with four other cubes, resulting in a layer



parallel to the (001) plane (Figures 1 and 2). Bismuth is coordinated as  $\psi^1$ -square pyramid [BiO<sub>4</sub>]<sup>5-</sup> by



four oxygen atoms (*d*(Bi–O) = 224.2(4) pm), which are connected via four vertices to infinite layers

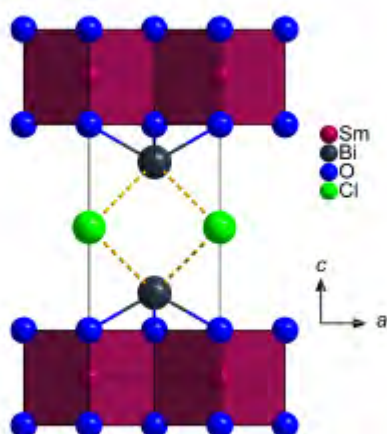


sandwiching the layers from both sides. The Cl<sup>-</sup> anions are not efficiently connected to the Bi<sup>3+</sup> cations (*d*(Cl<sup>-</sup>⋯Bi) = 336.7(1) pm), but located in the gaps between the lone pairs at the Bi<sup>3+</sup> centres.

**References**

- [1] M. Schmidt, H. Oppermann, C. Henning, R. W. Henn, E. Gmelin, N. Söger, *Z. Anorg. Allg. Chem.* **2000**, 626, 125–135.  
 [2] F. C. Goerigk, Th. Schleid, *Z. Anorg. Allg. Chem.* **2019**, 645, 1079–1084.  
 [3] F. C. Goerigk, *Doctoral Dissertation*, Univ. Stuttgart **2021**.

Extended unit cell of SmBi<sub>2</sub>O<sub>4</sub>Cl.



[SmO<sub>8</sub>]<sup>13-</sup> cube (left) and Bi–O layer (right).

