Poster

Closing Some Gaps of Knowledge: Single Crystals of $Nd_2[Sb_4O_8]Cl_2$

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The neodymium(III) oxidoantimonate(III) chloride $NdSb_2O_4Cl$ is accessible from solid-state reactions of Sb_2O_3 with Nd_2O_3 and $NdCl_3$ at 750 °C for two days. It crystallizes like $SmSb_2O_4Cl$ and $EuSb_2O_4Cl$ [1] in the centrosymmetric tetragonal space group $P4/ncc$ with the lattice parameters a = 793.85(4) pm and c = 1767.56(12) pm (c/a = 2.227) with Z = 8 (CSD number: 2350399). Thus it can also be described with the crystal-chemical formula $Nd_2[Sb_4O_8]Cl_2$ for Z = 4, for comprising isolated $[Sb_4O_8]^{4-}$ rings. This structural motif has some very close similarities to the well-known series of non-centrosymmetric $LnSb_2O_4Cl$ representatives (Ln = Gd – Lu) [2], crystallizing in the tetragonal space group $P42_12$. The crystal structure contains two positions for the Nd^{3+} cations (Nd1 at 4*a*: ¾, ¼, ¼ and Nd2 at 4*c*: ¼, ¼, 0.26038(9)), two partially occupied Sb^{3+} cations (Sb1 at 16*g*: 0.9938(3), 0.0575(3), 0.10463(9) and Sb2 at 16*g*: 0.0402(16), 0.9787(16), 0.1046(4)) and two O^{2-}-anion sites (O1 at 16*g*: 0.0077(16), 0.6782(16), 0.1784(8) and O2 at 16*g*: –0.0009(16), 0.2910(16), 0.1619(8)) as well as two Cl^--anion sites (Cl1 at 4*b*: ¾, ¼, 0 and Cl2 at 4*c*: ¼, ¼, 0.4892(5)). All Nd^{3+} cations have eight oxygen atoms as nearest neighbors arranged as square prisms $[NdO_8]^{13-}$, which are connected to layers by four parallel edges according to $^{2}_{\infty}\{[NdO^{e}_{8/2}]^{5-}\}$ with a two-dimensional fluorite-like topology. The Sb^{3+} cations together with three oxygen atoms each and their lone-pair of electrons form ψ^1-tetrahedra $[SbO_3]^{3-}$. Four of these $[SbO_3]^{3-}$ entities are vertex-connected to $^{0}_{\infty}\{[Sb_4O_8]^{4-}\}$ rings with four bridging and four terminal oxygen atoms. All three centrosymmetric representatives (Ln = Nd, Sm and Eu), in contrast to the series of non-centrosymmetric ones (Ln = Gd – Lu), have a doubled lattice parameter c. The antimony positions reflect a severe stacking fault order, which is why there are two partially occupied antimony positions, 77 % for Sb1 and 23 % for Sb2.

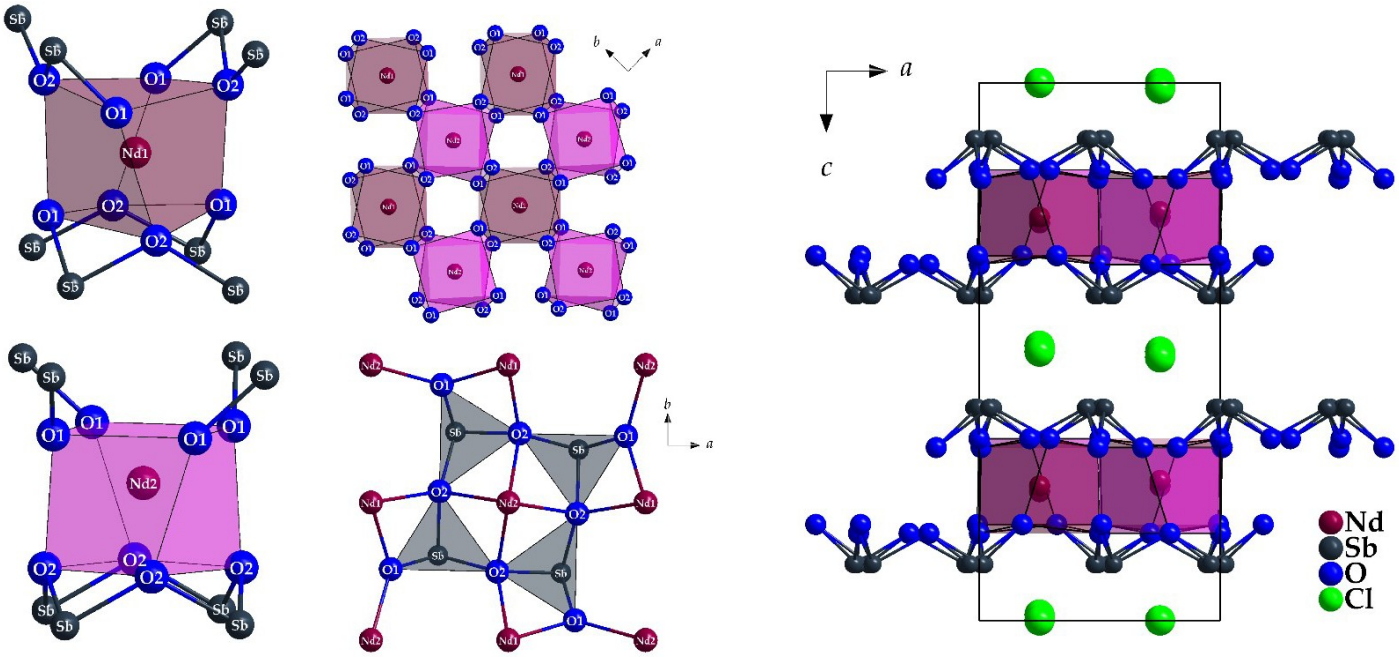

Figure 1. The two distinct $[NdO_8]^{13-}$ polyhedra with their antimony decoration (*left*), infinite layers of edge-sharing $[NdO_8]^{13-}$ polyhedra (*mid, top*), an isolated ring $[Sb_4O_8]^{4-}$ of four vertex-linked ψ^1-tetrahedra $[SbO_3]^{3-}$ with neodymium decoration (*mid, bottom*) and the extended tetragonal unit cell of $NdSb_2O_4Cl$ as viewed along [010] (*right*).

[1] Locke, R. J. C., Schleid, Th. (2022). *Z. Anorg. Allg. Chem.* **648**, e202200118.

[2] Locke, R. J. C., Goerigk, F. C., Schleid, Th. (2022). *Z. Naturforsch.* **77b**, 495.