# Crystal structure of dineodymium antimonide, $Nd_2Sb$

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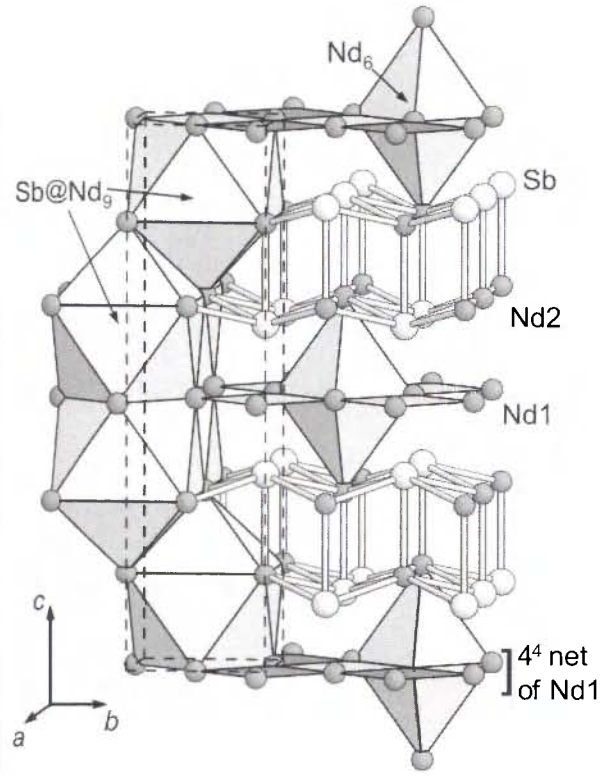
Received October 24, 2005, accepted and available on-line December 5, 2005; CSD no. 409859




**Abstract**

$Nd_2Sb$, tetragonal, *I4/mmm* (no. 139), $a = 4.5134(1)$ Å, $c = 17.5823(5)$ Å, $V = 358.2$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.025$, $wR_{ref}(F^2) = 0.057$, $T = 298$ K.

**Source of material**

$Nd_2Sb$ was synthesized from the elements with an excess of neodymium metal (ratio Nd:Sb = 4:1) in a sealed tantalum ampoule at 1915 K for one hour. The cooling process (cooling rate 25 K/h) was stopped temporarily at 1400 K for 48 h. Single crystals of sufficient quality for X-ray diffraction were isolated from the solidified mixture of $Nd_2Sb$ and Nd.

**Discussion**

$Nd_2Sb$ belongs to the *tI*12 structure type of $La_2Sb$ as was deduced by Borzone et al. [1] from powder diffraction data. The structure is build up by condensed mono-capped square antiprisms $SbNd_9$, $d$(Sb—Nd1) = 3.3125(4) Å (4×); $d$(Sb—Nd2) = 3.2174(6) Å (1×), 3.2726(2) Å (4×). The nearest neighbors of the Nd2 atoms are five Sb atoms arranged at the corners of a square pyramid, forming NaCl type fragments, which are also a distinct feature of $Sc_2Sb$ and related structures [2-4]. The short Nd1—Nd1′ distances of 3.1915(1) Å in the non-capped square of the $SbNd_9$ polyhedra indicate additional Nd—Nd interactions in the $4^4$ nets of Nd1. Obviously this leads to the large $c/a$ ratio ($3.896 >> 3.414 = 2+2^{1/2}$) compared to e. g. $Eu_4Sb_2O$ [5] ($K_2NiF_4$ structure type). In accordance with this observation, the final difference Fourier synthesis gave no evidence for an interstitial atom in the quasi-octahedral $Nd_6$ cavities (see also [6]).

**Table 1.** Data collection and handling.

| | |
|---|---|
| Crystal: | metallic dark silver block, size 0.05 × 0.08 × 0.15 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 357.60 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker AXS SMART APEX CCD, $\omega$ |
| $2\theta_{max}$: | 84.98° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 6194, 437 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 436 |
| $N(param)_{refined}$: | 11 |
| Programs: | SHELXTL [7], ATOMS [8] |

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Nd(1) | 4*c* | 0 | ½ | 0 | 0.0097(2) | 0.0166(2) | 0.0105(2) | 0 | 0 | 0 |
| Nd(2) | 4*e* | 0 | 0 | 0.17910(2) | 0.0094(1) | $U_{11}$ | 0.0085(1) | 0 | 0 | 0 |
| Sb | 4*e* | 0 | 0 | 0.36209(3) | 0.0089(1) | $U_{11}$ | 0.0093(2) | 0 | 0 | 0 |

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*Acknowledgment.* The authors gratefully acknowledge the help of Mrs. S. Prill-Diemer for carrying out the synthesis.

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