

## C-type Nd<sub>2</sub>Se<sub>3</sub>

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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{Nd}-\text{Se}) = 0.0005$  Å;  $R$  factor = 0.026;  $wR$  factor = 0.060; data-to-parameter ratio = 31.4.

The title compound, neodymium sesquiselenide, is isotopic with the other known rare-earth metal(III) selenides  $M_2\text{Se}_3$  ( $M = \text{La}-\text{Pr}$  and  $\text{Sm}-\text{Lu}$ ) with the cubic C-type structure. It adopts a cation-defective  $\text{Th}_3\text{P}_4$ -type arrangement with close to 8/9 of the unique neodymium-cation site occupied, leading to the composition  $\text{Nd}_{2.667}\text{Se}_4$  ( $Z = 4$ ) or  $\text{Nd}_2\text{Se}_3$  ( $Z = 5.333$ ), respectively. The  $\text{Nd}^{3+}$  cations are thus surrounded by eight selenide anions, forming trigonal  $[\text{NdSe}_8]^{13-}$  dodecahedra, whereas the  $\text{Se}^{2-}$  anions exhibit a sixfold coordination, but due to the under-occupation of neodymium, each one is statistically surrounded by only 5.333 cations. The crystal studied was a merohedral twin with a 0.31 (6):0.69 (6) domain ratio.

### Related literature

For the structural family with the cation-defective  $\text{Th}_3\text{P}_4$ -type arrangement, see: Pardo *et al.* (1963); Flahaut *et al.* (1965); Lashkarev & Paderno (1965). For the rare-earth sesquiselenides  $M_2\text{Se}_3$  with  $M = \text{La}-\text{Pr}$  and  $\text{Sm}-\text{Lu}$ , see: Grundmeier & Urland (1995); Folchnandt (1997); Folchnandt & Schleid (2001); Folchnandt *et al.* (2004).

### Experimental

#### Crystal data

$\text{Nd}_{2.667}\text{Se}_4$	$Z = 4$
$M_r = 700.48$	Mo $K\alpha$ radiation
Cubic, $I\bar{4}3d$	$\mu = 40.39$ mm <sup>-1</sup>
$a = 8.8632$ (6) Å	$T = 293$ K
$V = 696.26$ (8) Å <sup>3</sup>	$0.03 \times 0.03 \times 0.02$ mm

#### Data collection

Stoe IPDS-I diffractometer	8964 measured reflections
Absorption correction: numerical ( <i>X-SHAPE</i> ; Stoe & Cie, 1999)	220 independent reflections
$T_{\min} = 0.305$ , $T_{\max} = 0.401$	214 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.065$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	$\Delta\rho_{\text{max}} = 1.01$ e Å <sup>-3</sup>
$wR(F^2) = 0.060$	$\Delta\rho_{\text{min}} = -2.11$ e Å <sup>-3</sup>
$S = 1.22$	Absolute structure: Flack (1983), 92 Friedel pairs
220 reflections	Flack parameter: 0.31 (6)
7 parameters	

**Table 1**

Selected bond lengths (Å).

Nd–Se <sup>i</sup> (4×)	2.9675 (5)	Nd–Se (4×)	3.1732 (6)
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 Symmetry codes: (i)  $-x + \frac{1}{2}, -y, z + \frac{1}{2}$ .

Data collection: *DIF4* (Stoe & Cie, 1992); cell refinement: *DIF4*; data reduction: *REDU4* (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2064).

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