Crystal structure of trisodium dineodymium nonanitrate, $Na_3[Nd_2(NO_3)_9]$

S. Stockhause

Universität Hannover, Institut für Anorganische Chemie, Callinstr. 9, D-30167 Hannover, Germany

and G. Meyer

Universität zu Köln, Institut für Anorganische Chemie, Greinstr. 6, D-50939 Köln, Germany

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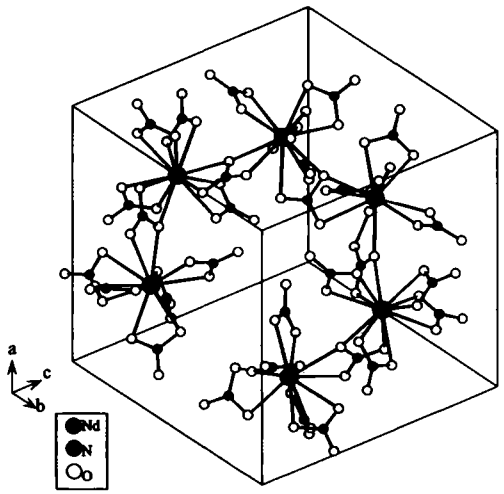

Source of material: $Na_3[Nd_2(NO_3)_9]$ crystallizes from a melt of $Nd(NO_3)_3$ and $NaNO_3$ (molar ratio 1:3) by slow cooling from 588 K to room temperature in a silica boat under strict exclusion of oxygen and moisture.

In the crystal structure of $Na_3[Nd_2(NO_3)_9]$ Nd^{3+} is surrounded by six bidentate nitrate ligands of which three are bridging to neigh- bouring Nd^{3+} ions. This results in a branched folded chain. The Na^+ ions occupy cavities in the structure. $Na_3[Nd_2(NO_3)_9]$ is isotypic with a number of analogous potassium, ammonium and rubidium nitrates (see refs. 1-3).

$N_9Na_3Nd_2O_{27}$, cubic, $P4_132$ (No. 213), a =13.1279(8) Å, V =2262.5 Å^3, Z =4, $R(F)$ =0.041, $R_w(F^2)$ =0.067.

Table 1. Parameters used for the X-ray data collection

Crystal:	violet, irregular, size 0.1 x 0.1 x 0.1 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	44.57 cm^{-1}
Diffractometer:	Siemens-Stoe AED 2
Scan mode:	ω/2θ, background-peak-background
$T_{measurement}$:	293 K
$2\theta_{max}$:	52°
$N(hkl)_{unique}$:	755
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	64
Programs:	SHELXS-86, SHELXL-93

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Table 2. Final 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	8c	0.71181(4)	x	x	0.0265(2)	U_{11}	U_{11}	0.0011(3)	U12	U_{12}
Na	12d	5/8	0.3296(3)	y+1/4	0.114(7)	0.048(3)	U_{22}	–0.005(3)	–0.003(3)	$-U_{12}$
N(1)	12d	5/8	0.4945(6)	y+1/4	0.025(7)	0.030(4)	U_{22}	0.000(3)	0.006(5)	$-U_{12}$
O(1)	24e	0.7651(4)	0.5860(5)	0.4119(5)	0.034(4)	0.046(5)	0.023(4)	0.006(3)	0.001(3)	–0.004(3)
O(2)	12d	5/8	0.5638(4)	y+1/4	0.042(6)	0.027(3)	U_{22}	–0.002(3)	–0.008(4)	$-U_{12}$
N(2)	24e	0.6318(7)	0.6026(7)	0.1114(7)	0.043(6)	0.039(6)	0.033(5)	0.009(5)	–0.003(4)	–0.002(4)
O(3)	24e	0.6770(6)	0.6538(5)	0.1761(6)	0.068(6)	0.043(4)	0.048(5)	–0.007(4)	–0.006(4)	–0.018(4)
O(4)	24e	0.5506(5)	0.5556(5)	0.1329(4)	0.037(5)	0.042(5)	0.034(4)	–0.006(4)	0.003(4)	–0.008(3)
O(5)	24e	0.6681(5)	0.5916(5)	0.0223(5)	0.044(4)	0.037(4)	0.033(4)	–0.003(3)	0.003(3)	0.002(3)