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Crystal structure of disodium praseodymium pentanitrate monohydrate, $Na_2[Pr(NO_3)_5] \cdot H_2O$

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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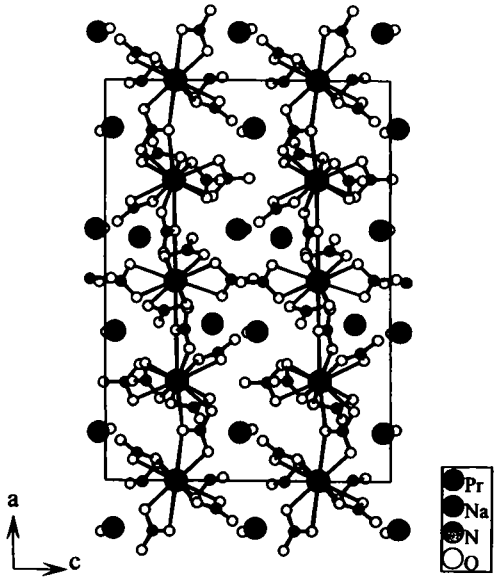

Source of material: $Na_2[Pr(NO_3)_5] \cdot H_2O$ crystallizes from a solution of Pr_6O_{11} and $NaNO_3$ in conc. HNO_3 upon slow evaporation in a desiccator over solid KOH. It is also obtained from a solution of $Na_3Nd_2(NO_3)_9$ in acetonitrile by isothermic evaporation in a slow stream of argon.

In the crystal structure of $Na_2[Pr(NO_3)_5] \cdot H_2O$ Pr^{3+} is (as Nd^{3+} in the isotypic $Na_2[Nd(NO_3)_5](H_2O)$, see ref.1) surrounded by six bidentate nitrate ligands of which two are bridging to neighbouring Pr^{3+} ions. The Na^+ ions and the water molecules are located between these chains.

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

Crystal:	greenish, irregular, size 0.1 x 0.1 x 0.1 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	37.65 cm^{-1}
Diffractometer:	Siemens-Stoe AED 2
Scan mode:	ω/2θ, background-peak-background
$T_{measurement}$:	293 K
$2\theta_{max}$:	42°
$N(hkl)_{unique}$:	2751
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	224
Programs:	SHELXS-86, SHELXL-93

$H_2N_5Na_2O_{16}Pr$, monoclinic, $P12/c1$ (No. 13), a =21.309(6) Å, b =7.910(3) Å, c =15.16(1) Å, β =90.72(3)°, V =2555.1 $Å^3$, Z =8, $R(F)$ =0.053, $R_w(F^2)$ =0.099.

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{iso}
N(1)	4g	0.1833(8)	0.488(2)	0.313(1)	0.016(4)
O(11)	4g	0.2048(6)	0.388(2)	0.3695(8)	0.025(4)
O(12)	4g	0.1925(6)	0.455(2)	0.2328(8)	0.025(4)
O(13)	4g	0.1543(7)	0.614(2)	0.3318(9)	0.032(4)
N(2)	4g	0.4243(8)	0.845(2)	0.209(1)	0.028(4)
O(21)	4g	0.4351(6)	0.946(2)	0.1514(8)	0.017(4)
O(23)	4g	0.3939(7)	0.713(2)	0.1909(9)	0.037(4)
O(22)	4g	0.4400(6)	0.872(2)	0.2889(8)	0.024(4)
N(3)	4g	0.0029(7)	0.480(2)	0.369(1)	0.024(4)
O(31)	4g	0.9567(6)	0.451(2)	0.3165(8)	0.024(4)
H(032)	4g	0.0438(7)	0.362(2)	0.3686(8)	0.031(4)
O(33)	4g	0.0082(7)	0.602(2)	0.4137(9)	0.038(4)
N(4)	4g	0.0690(8)	0.984(3)	0.112(1)	0.026(5)
O(41)	4g	0.0528(7)	0.137(2)	0.0971(8)	0.026(4)
O(43)	4g	0.1003(7)	0.907(2)	0.0535(9)	0.035(4)
O(42)	4g	0.0547(6)	0.912(2)	0.1781(8)	0.022(4)
N(5)	4g	0.2455(9)	0.288(3)	0.070(1)	0.033(5)
O(51)	4g	0.2001(6)	0.203(2)	0.0985(8)	0.021(3)
O(52)	4g	0.2893(7)	0.320(2)	0.1214(8)	0.028(4)
O(53)	4g	0.2448(7)	0.665(2)	0.492(1)	0.044(5)
N(6)	4g	0.2493(8)	0.853(2)	0.144(1)	0.022(4)
O(61)	4g	0.2931(6)	0.960(2)	0.1414(8)	0.027(4)
O(63)	4g	0.2486(7)	0.725(2)	0.0955(9)	0.040(4)
O(62)	4g	0.2062(6)	0.890(2)	0.1936(8)	0.019(3)
N(7)	4g	0.6806(8)	0.979(2)	0.102(1)	0.022(4)
O(71)	4g	0.6979(6)	0.130(2)	0.0916(8)	0.021(4)
O(73)	4g	0.6471(7)	0.911(2)	0.0431(9)	0.032(4)
O(72)	4g	0.6971(7)	0.901(2)	0.1692(9)	0.032(4)
N(8)	4g	0.3779(7)	0.345(2)	0.2816(8)	0.013(4)
O(81)	4g	0.3752(7)	0.200(2)	0.2513(9)	0.015(3)
O(82)	4g	0.4305(7)	0.418(2)	0.2913(8)	0.027(4)
O(83)	4g	0.3302(7)	0.430(2)	0.2985(8)	0.030(4)
N(9)	4g	0.5034(8)	0.250(2)	0.444(1)	0.020(4)
O(91)	4g	0.5435(6)	0.306(2)	0.3883(8)	0.027(4)
O(92)	4g	0.4605(7)	0.155(2)	0.4118(8)	0.032(4)
O(93)	4g	0.5051(7)	0.706(2)	0.0213(9)	0.029(4)
N(10)	4g	0.1253(7)	0.049(2)	0.3347(9)	0.017(4)
O(102)	4g	0.0729(7)	0.990(2)	0.3619(9)	0.029(4)
O(103)	4g	0.1746(7)	0.001(2)	0.3732(8)	0.025(4)
O(101)	4g	0.1256(6)	0.152(2)	0.2737(7)	0.013(4)
O(1W)	4g	0.3706(8)	0.486(2)	0.503(1)	0.035(4)
O(2W)	4g	0.1280(7)	0.470(2)	0.5174(8)	0.031(4)

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Table 3. 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}
Pr(1)	2*e*	0	0.1713(3)	1/4	0.007(1)	0.019(1)	0.026(1)	0	0.0011(9)	0
Pr(2)	2*f*	1/2	0.1463(3)	1/4	0.005(1)	0.022(2)	0.028(1)	0	0.0019(9)	0
Pr(3)	4*g*	0.24905(7)	0.1678(2)	0.25504(9)	0.0041(7)	0.0188(9)	0.0241(8)	0.0008(8)	0.0001(6)	–0.0002(8)
Na(1)	4*g*	0.1272(4)	0.660(1)	0.1586(5)	0.009(4)	0.026(6)	0.039(5)	0.003(4)	–0.008(4)	–0.004(5)
Na(2)	4*g*	0.1196(5)	0.763(1)	0.4739(5)	0.036(6)	0.041(7)	0.034(5)	0.005(5)	–0.004(4)	0.004(5)
Na(3)	4*g*	0.3724(4)	0.813(1)	0.0347(5)	0.031(6)	0.039(7)	0.034(5)	–0.002(5)	0.000(4)	–0.001(5)
Na(4)	4*g*	0.3917(5)	0.663(1)	0.3784(6)	0.074(8)	0.027(6)	0.046(6)	–0.002(6)	0.006(5)	0.008(5)

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