

Crystal structure of tetraqua gadolinium trinitrate monohydrate, $[\text{Gd}(\text{NO}_3)_3(\text{H}_2\text{O})_4] \cdot \text{H}_2\text{O}$

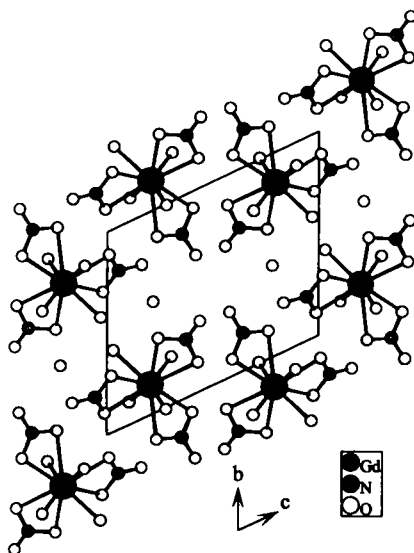
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Source of material: $[\text{Gd}(\text{NO}_3)_3(\text{H}_2\text{O})_4](\text{H}_2\text{O})$ crystallizes from a solution of Gd_2O_3 in conc. HNO_3 upon slow evaporation in a desiccator over solid KOH as colourless small rods.

The crystal structure of gadolinium nitrate pentahydrate consists of $[\text{Gd}(\text{NO}_3)_3(\text{H}_2\text{O})_4]$ units between which the fifth water molecule is located as crystal water. Isolated $[\text{Gd}(\text{NO}_3)_3(\text{H}_2\text{O})_4]$ units are also known from $\text{M}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, $\text{M} = \text{Gd}, \text{Nd}$ (see refs. 1, 2).

Table 2. Final atomic coordinates and displacement parameters (in \AA^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Gd	2i	0.25403(5)	0.15068(4)	0.20541(3)	0.0291(2)	0.0293(2)	0.0257(2)	-0.0061(1)	0.0002(1)	-0.0122(2)
N(1)	2i	0.032(1)	0.2160(8)	-0.0550(7)	0.041(3)	0.040(4)	0.032(3)	-0.011(3)	-0.005(3)	-0.015(3)
O(11)	2i	-0.050(1)	0.2830(8)	0.0220(6)	0.041(3)	0.044(3)	0.039(3)	-0.004(3)	0.003(2)	-0.022(3)
O(12)	2i	0.205(1)	0.1168(8)	-0.0106(7)	0.042(3)	0.049(4)	0.047(3)	0.004(3)	-0.009(3)	-0.027(3)
O(13)	2i	-0.048(1)	0.241(1)	-0.1637(8)	0.058(4)	0.067(5)	0.047(4)	-0.005(4)	-0.022(3)	-0.033(4)
N(2)	2i	0.476(1)	-0.1869(8)	0.3556(8)	0.038(3)	0.034(3)	0.040(4)	-0.001(3)	-0.008(3)	-0.016(3)
O(21)	2i	0.440(1)	-0.0833(8)	0.4059(7)	0.056(4)	0.041(3)	0.038(3)	-0.004(3)	-0.007(3)	-0.023(3)
O(22)	2i	0.397(1)	-0.1389(8)	0.2362(7)	0.045(3)	0.048(4)	0.040(3)	-0.009(3)	-0.005(3)	-0.022(3)
O(23)	2i	0.578(2)	-0.3203(9)	0.4191(9)	0.088(6)	0.038(4)	0.066(5)	0.014(4)	-0.018(4)	-0.019(4)
N(3)	2i	-0.022(1)	0.2873(9)	0.3753(8)	0.042(4)	0.047(4)	0.042(4)	-0.006(3)	0.010(3)	-0.030(3)
O(31)	2i	-0.007(1)	0.3592(8)	0.2426(7)	0.059(4)	0.045(4)	0.034(3)	-0.001(3)	0.003(3)	-0.011(3)
O(32)	2i	0.090(1)	0.1489(7)	0.4312(6)	0.051(3)	0.039(3)	0.038(3)	-0.011(3)	0.007(3)	-0.019(3)
O(33)	2i	-0.137(2)	0.345(1)	0.4404(9)	0.078(6)	0.064(5)	0.059(4)	0.000(4)	0.019(4)	-0.034(4)
O(1W)	2i	0.472(1)	0.2388(7)	0.3064(6)	0.059(4)	0.040(3)	0.037(3)	-0.019(3)	-0.006(3)	-0.017(3)
O(2W)	2i	-0.017(1)	-0.0064(7)	0.2804(6)	0.045(3)	0.039(3)	0.031(3)	-0.010(3)	0.002(2)	-0.013(2)
O(3W)	2i	0.300(1)	0.4040(7)	0.0308(7)	0.045(3)	0.035(3)	0.040(3)	-0.006(3)	0.001(3)	-0.012(2)
O(4W)	2i	0.5932(9)	0.1148(8)	0.1061(7)	0.033(3)	0.052(4)	0.052(4)	-0.007(3)	0.002(3)	-0.031(3)
O(5W)	2i	0.500(2)	0.4508(8)	-0.2187(7)	0.090(6)	0.039(4)	0.041(4)	-0.012(4)	0.004(4)	-0.019(3)

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

Crystal:	colorless, irregular, size 0.1 x 0.1 x 0.1 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 \AA)
μ :	53.90 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	100 exposures, $\Delta\phi = 2^\circ$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	56.3°
$N(hkl)_{\text{unique}}$:	2662
Criterion for I_0 :	$I_0 > 2\sigma(I_0)$
$N(\text{param})_{\text{refined}}$:	164
Programs:	SHELXS-86, SHELXL-93

$\text{GdH}_{10}\text{N}_3\text{O}_{14}$, triclinic, $P\bar{1}$ (No. 2), $a = 6.692(1) \text{ \AA}$, $b = 9.588(2) \text{ \AA}$, $c = 10.622(2) \text{ \AA}$, $\alpha = 63.70(1)^\circ$, $\beta = 84.68(1)^\circ$, $\gamma = 76.19(1)^\circ$, $V = 593.3 \text{ \AA}^3$, $Z = 2$, $R(F) = 0.049$, $R_w(F^2) = 0.125$.

References

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