Crystal structure of tetraaqua gadolinium trinitrate monohydrate, $[Gd(NO_3)_3(H_2O)_4] \cdot H_2O$

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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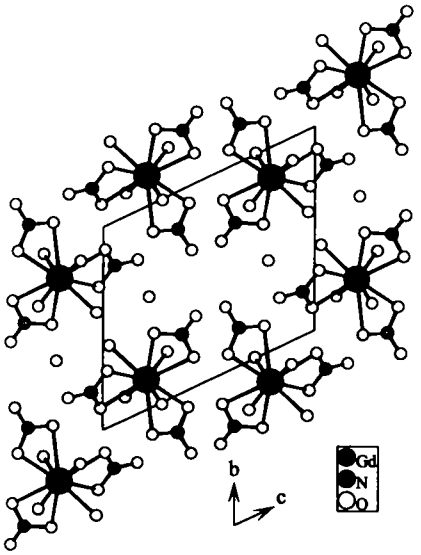

Source of material: $[Gd(NO_3)_3(H_2O)_4](H_2O)$ crystallizes from a solution of Gd_2O_3 in conc. HNO_3 upon slow evaporation in a desiccator over solid KOH as colourless small rods.

The crystal structure of gadolinium nitrate pentahydrate consists of $[Gd(NO_3)_3(H_2O)_4]$ units between which the fifth water molecule is located as crystal water. Isolated $[Gd(NO_3)_3(H_2O)_4]$ units are also known from $M(NO_3)_3 \cdot 6H_2O$, M = Gd, Nd (see refs. 1, 2).

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_α radiation (0.71073 Å)
μ:	53.90 cm^{-1}
Diffractometer:	Stoe IPDS
Scan mode:	100 exposures, $\Delta\varphi = 2°$
$T_{measurement}$:	293 K
$2\theta_{max}$:	56.3°
$N(hkl)_{unique}$:	2662
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	164
Programs:	SHELXS-86, SHELXL-93

$GdH_{10}N_3O_{14}$, triclinic, $P\bar{1}$ (No. 2), a =6.692(1) Å, b =9.588(2) Å, c =10.622(2) Å, α =63.70(1)°, β =84.68(1)°, γ=76.19(1)°, V =593.3 Å^3, Z=2, $R(F)$ =0.049, $R_w(F^2)$ =0.125.

References

1. Ma, H.; Gao, S.; Zupci, Y.: Crystal structure of Gadolinium(III)nitrate-hexa-hydrate. Wuji Huaxue Xuebao **7** (1991) 351-353.
2. Rogers, D. J; Taylor, N. J.; Toogood, G. E.: Tetraaquatrinitratoneodymium(III)-dihydrate. Acta Crystallogr. C**39** (1983) 939-941.
3. Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Large Structures. Acta Crystallogr. A**46** (1990) 467-473.
4. Sheldrick, G. M.: SHELXL-93, a program for refining crystal structures. University of Göttingen, Germany 1993.

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}
Gd	2*i*	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)	2*i*	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)	2*i*	−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)	2*i*	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)	2*i*	−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)	2*i*	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)	2*i*	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)	2*i*	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)	2*i*	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)	2*i*	−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)	2*i*	−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)	2*i*	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)	2*i*	−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)	2*i*	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)	2*i*	−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)	2*i*	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)	2*i*	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)	2*i*	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)