Crystal structure of triholmium pentagallium dodecaoxide, $Ho_3Ga_2(GaO_4)_3$ and of tridysprosium pentagallium dodecaoxide, $Dy_3Ga_2(GaO_4)_3$

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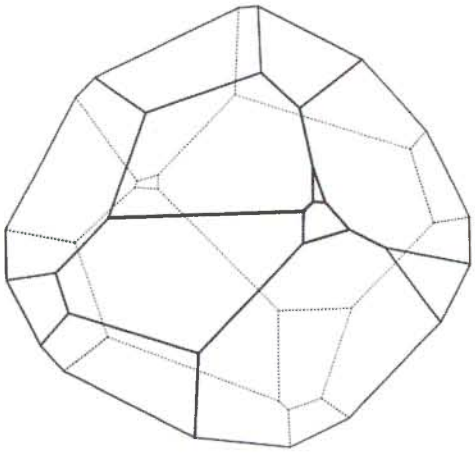
Abstract

$Ga_5Ho_3O_{12}$, cubic, $Ia\bar{3}d$ (No. 230), $a = 12.290(2)$ Å, $V = 1856.3$ Å^3, $Z = 8$, $R_{gt}(F) = 0.018$, $R_w(F^2) = 0.029$, $T = 300$ K.

$Dy_3Ga_5O_{12}$, cubic, $Ia\bar{3}d$ (No. 230), $a = 12.306(1)$ Å, $V = 1863.6$ Å^3, $Z = 8$, $R_{gt}(F) = 0.017$, $R_w(F^2) = 0.026$, $T = 300$ K.

1. Triholmium pentagallium dodecaoxide, $Ho_3Ga_2(GaO_4)_3$ (holmium gallium garnet)



Source of material

Single crystals of holmium gallium garnet were grown by chemical vapour transport in a closed quartz ampoule. Chlorine was used as transporting agent and a mixture of ZnO (6.0 mmol), Ga_2O_3 (6.0 mmol) and Ho_2O_3 (0.3 mmol) as source material. After 3 days of back transport chemical transport (1323 K → 1073 K) was continued for 18 days. Zinc gallium spinel and yellow crystals of holmium gallium garnet were deposited in the crystallization zone.

Discussion

$Ho_3Ga_5O_{12}$ has the YAG-type structure as many other RE-Ga-garnets, which are already known [1]. From powder data the lattice constant $a = 12.281$ Å is reported [2]. In our sample the small crystals, which were suitable for the X-ray investigation, showed no well developed faces, but on some crystals faces of type (211) were observed. Therefore the {211}-form was used to approximate the shape of the crystal. The figure shows the shape as it was used in the numerical absorption correction procedure (programs X-SHAPE [3] and X-RED [4]). The R_{int} value is 0.0761 without absorption correction. A numerical absorption correction was necessary to obtain reasonable anisotropic displacement parameters. Since these parameters strongly depend on the absorption correction, they have to be inspected critically.The most important interatomic distances are: Ho–O 2.340(3) Å and 2.437(4) Å, Ga(1)–O 1.995(3) Å, Ga(2)–O 1.845(3) Å. 3 forbidden weak reflections of type hhl with $I/\sigma(I)<6$ were neglected.

Table 1. Data collection and handling.

Crystal:	light yellow, ellipsoidal shape, size 0.088 x 0.107 x 0.132 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	396 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 160 exposures, $\Delta\varphi = 1.8°$
$2\theta_{max}$:	56.28°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9501, 197
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 149
$N(param)_{refined}$:	18
Programs:	X-SHAPE [3], X-RED [4], SHELXL-93 [5], MOPLO [6], CIF2SX [7]

Table 2. 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}
Ho(1)	24*c*	0	1/4	1/8	0.0061(2)	U_{11}	0.0046(2)	0.0007(2)	0	0
Ga(1)	16*a*	0	0	0	0.0049(2)	U_{11}	U_{11}	–0.0002(3)	U_{12}	U_{12}
Ga(2)	24*d*	0	1/4	3/8	0.0045(3)	U_{11}	0.0031(4)	0	0	0
O(1)	96*h*	–0.0274(3)	0.0552(3)	0.1502(3)	0.005(2)	0.010(2)	0.006(2)	–0.001(1)	0.001(1)	0.000(1)

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2. Tridysprosium pentagallium dodecaoxide, $Dy_3Ga_2(GaO_4)_3$ (dysprosium gallium garnet)

Source of material

Single crystals of dysprosium gallium garnet were grown by chemical vapour transport in a closed quartz ampoule using chlorine as transporting agent. The garnet was synthesized by back transport (2 days) in the reaction ampoule from stoichiometric amounts of Dy_2O_3 and Ga_2O_3. After 7 days of chemical transport (1323 K → 1073 K), Ga_2O_3 and yellow to light brownish single crystals of dysprosium gallium garnet were obtained.

Discussion

$Dy_3Ga_5O_{12}$ has the YAG-type structure as many other RE-Ga-garnets, which are already known [1]. From powder data the lattice constant a = 12.307 Å is reported [8]. The irregular shape of the crystal investigated by us was approximated by an irregular polyhedron with 20 faces (no figure supplied for this crystal). The most important interatomic distances are : Dy–O 2.347(2) Å and 2.444(2) Å, Ga(1)–O 1.994(2) Å, Ga(2)–O 1.845(2) Å.

Table 3. Data collection and handling.

Crystal:	light brownish, irregular shape, size 0.08 x 0.12 x 0.18 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	380 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, 150 exposures, $\Delta\varphi = 1.5°$
$2\theta_{max}$:	56.2°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8422, 197
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 160
$N(param)_{refined}$:	18
Programs:	X-SHAPE [3], X-RED [4], SHELXL-93 [5], CIF2SX [7]

Table 4. 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}
Dy(1)	24*c*	0	1/4	1/8	0.0059(2)	U_{11}	0.0044(2)	0.0008(1)	0	0
Ga(1)	16*a*	0	0	0	0.0050(2)	U_{11}	U_{11}	–0.0003(2)	U_{12}	U_{12}
Ga(2)	24*d*	0	1/4	3/8	0.0047(2)	U_{11}	0.0032(3)	0	0	0
O(1)	96*h*	–0.0278(2)	0.0549(2)	0.1499(2)	0.006(1)	0.009(1)	0.006(1)	–0.0014(8)	0.0014(8)	0.0004(8)

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