

Rietveld refinement of Y_2GeO_5 Eric M. Rivera-Muñoz^{a*} and Lauro Bucio^b

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Key indicators: powder X-ray study; $T = 300$ K; mean $\sigma(Y-O) = 0.009$ Å; R factor = 0.053; wR factor = 0.069; data-to-parameter ratio = 5.5.

Y_2GeO_5 (yttrium germanium pentaoxide) was synthesized by solid-state reaction at 1443 K. The arrangement, which has monoclinic symmetry, is isostructural with Dy_2GeO_5 and presents two independent sites for the Y atoms. Around these atoms there are distorted six-coordinated YO_6 octahedra and seven-coordinated YO_7 pentagonal bipyramids. The YO_7 polyhedra are linked together, sharing their edges along a surface parallel to ab , forming a sheet. Each of these parallel sheets is interconnected by means of GeO_4 tetrahedra, sharing an edge (or vertex) on one side and a vertex (or edge) on the other adjacent side. Parallel sheets of YO_7 polyhedra are also interconnected by undulating chains of YO_6 octahedra along the c axis. These octahedra are joined together, sharing a common edge, to form the chain and share edges with the YO_7 polyhedra of the sheets.

Related literature

For the isotypic structure of Dy_2GeO_5 , see: Brixner *et al.* (1985). Different synthesis methods have been reported for this compound, including preparation by conventional r.f. magnetron sputtering (Minami *et al.*, 2003), solid-state reactions at high temperatures (Zhao *et al.*, 2003), MOCVD and LSMCD (Natori *et al.*, 2004). For bond-valence parameters, see: Brese & O'Keefe (1991), and for the bond-valence model, see: Brown (1981, 1992). For oxide phosphors, see: Minami *et al.* (2001, 2002, 2004). Data used to model the second phase present in the reaction product, $Y_2Ge_2O_7$, were taken from Redhammer *et al.* (2007). For related literature on technological applications, see: Fei *et al.* (2003).

Experimental

Crystal data

Y_2GeO_5	$c = 12.8795$ (2) Å
$M_r = 330.43$	$\beta = 101.750$ (3)°
Monoclinic, $I2/a$	$V = 901.66$ (3) Å ³
$a = 10.4706$ (2) Å	$Z = 8$
$b = 6.8292$ (1) Å	Cu $K\alpha$ radiation

$T = 300$ K
Specimen shape: flat sheet
 $20 \times 20 \times 0.2$ mm

Specimen prepared at 1443 K
Particle morphology: spherical,
white

Data collection

Bruker Advance D8 diffractometer
Specimen mounting: packed powder
sample container
Specimen mounted in reflection
mode

Scan method: step
 $2\theta_{\min} = 8.0$, $2\theta_{\max} = 80.0^\circ$
Increment in $2\theta = 0.02^\circ$

Refinement

$R_p = 0.053$
 $R_{wp} = 0.069$
 $R_{exp} = 0.024$
 $S = 2.90$
Wavelength of incident radiation:
1.540560 Å

Profile function: pseudo-Voigt
modified by Thompson *et al.*
(1987)
582 reflections
105 parameters

Data collection: *DIFFRAC/AT* (Siemens, 1993); cell refinement: *DICVOL91* (Boultif & Louër 1991); data reduction: *FULLPROF* (Rodríguez-Carvajal, 2006); method used to solve structure: coordinates taken from an isotypic compound (Brixner *et al.*, 1985); program(s) used to refine structure: *FULLPROF*; molecular graphics: *ATOMS* (Dowty, 2000); software used to prepare material for publication: *FULLPROF*.

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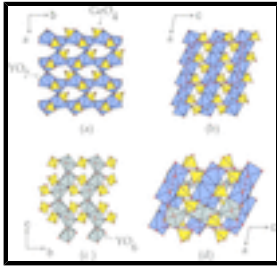
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2110).

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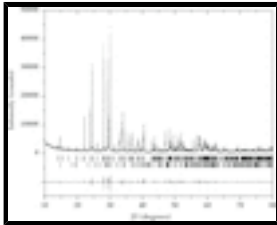
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