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CRYSTALLOGRAPHIC DATA FOR Er_2SiO_5 AND Y_2SiO_5 ¹

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Recent phase equilibria investigations of rare-earth oxide-silicon dioxide systems and their compounds have been the subject of studies by Warshaw and Roy (1961) and Toropov *et al.* (1961). Of specific interest to this paper are the compounds Er_2SiO_5 and Y_2SiO_5 , data for which were reported by both sets of authors. However, a comparison of the powder x-ray diffraction data for these two compounds as given by Warshaw and Roy with that given by Toropov *et al.* for the identical compounds are not in agreement.

Recently, we have synthesized single crystals of Er_2SiO_5 and Y_2SiO_5 by solution growth from a molten $\text{Li}_2\text{O} \cdot 2\text{MoO}_3$ solvent at approximately 1100° C. Spectrochemical analyses of the erbium compound showed only significant quantities of erbium and silicon with less than 0.1% Mo present. Confirmation of the formula was obtained by solid state synthesis of these compounds. This was accomplished by physically mixing powders

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TABLE 1. COMPARISON OF PHYSICAL PROPERTIES AND X-RAY POWDER DIFFRACTION DATA FOR Er_2SiO_5 OF TOROPOV *et al.* AND PRESENT AUTHORS

	Toropov <i>et al.</i>	Present ¹ authors
Optic figure	biaxial	biaxial
Refractive indices	$\gamma = 1.825$ $\alpha = 1.807$	$\gamma \cong 1.825$ $\alpha \cong 1.810$
2V (estimated)	88°	~90°
Density (measured $\text{g}\cdot\text{cm}^{-3}$)	6.8	6.87

Diffraction Data				
I	d(A)	I ²	d(A)	hkl
		M	6.075	002
		M	5.884	011
		VVW	5.566	110
		VVW	5.012	200
		W	4.380	$\bar{1}12, \bar{2}02$
12	4.08	M	4.048	$\bar{2}11$
46	3.92	VS	3.883	112
		VVW	3.628	211
41	3.55	S	3.531	202
		VVW	3.445	013
12	3.37	MW	3.337	020
54	3.15	S	3.129	$\bar{1}21$
82	3.03	VS	3.004	310
100	2.93	S	2.925	022
		VS	2.885	204
		W	2.792	220
30	2.67	M	2.653	$\bar{2}22$
		W	2.631	213
20	2.61	M	2.583	$\bar{1}23$
68	2.55	VS	2.533	114
43	2.42	M	2.412	123
36	2.27	MS	2.255	024
		MW	2.235	411
93	2.19	MW	2.186	031
		S	2.172	130
		W	2.035	$\bar{2}31$

¹ The x-ray powder diffraction data were obtained from Debye-Scherrer films using Cu $K\alpha$ ($\lambda = 1.5418 \text{ \AA}$) radiation.

² S=strong; VS=very strong; M=medium; MW=medium weak; MS=medium strong; W=weak; VW=very weak; and VVW=very very weak.

(the purity of these powders are 99.95 wt % Y_2O_3 , 99.9 wt % Er_2O_3 , and 99.95 wt % SiO_2) of the constituent oxides in their proper proportions, then pelletizing this mixture and firing the pellet at a temperature greater

TABLE 2. X-RAY DIFFRACTION DATA FOR Er_2SiO_5 AND Y_2SiO_5 BASED ON SINGLE CRYSTALS

	Er_2SiO_5	Y_2SiO_5
Color	Pink	Water clear
Lattice parameters		
a	$10.33 \pm 0.03 \text{ \AA}$	$10.34 \pm 0.02 \text{ \AA}$
b	$6.689 \pm 0.016 \text{ \AA}$	$6.689 \pm 0.015 \text{ \AA}$
c	$12.37 \pm 0.02 \text{ \AA}$	$12.38 \pm 0.03 \text{ \AA}$
β	$102^\circ 57'$	$102^\circ 32'$
Z	8	8
$\rho_0 (\text{g} \cdot \text{cm}^{-3})$	6.86	¹
$\rho_{x\text{-ray}} (\text{g} \cdot \text{cm}^{-3})$	7.057	4.55
Possible space groups	$Ic, I2/c$	$Ic, I2/c$

¹ Sample was too small for accurate determination.

than 1450°C . for 24 hr, in air, using a 60% Pt-40% Rh wound vertical tube furnace. The product obtained on air quenching was examined optically and by x-ray diffraction and found to be essentially a single phase, giving a diffraction pattern identical to the one obtained from powdered single crystals.

The diffraction data obtained in this study for Er_2SiO_5 and Y_2SiO_5 were found to differ from those reported by Warsaw and Roy for identical compounds. However, a comparison of physical properties and x-ray diffraction data (Table 1) for Er_2SiO_5 given by Toropov *et al.* and the present authors shows them to be the same with the exception that the weaker reflections were not observed by Toropov *et al.*

The crystallographic data for Er_2SiO_5 and Y_2SiO_5 are summarized in Table 2. Rotation, Weissenberg, and precession films were obtained from crystals of both compounds using $\text{Cu K}\alpha$ ($\lambda = 1.5418 \text{ \AA}$) and $\text{Mo K}\alpha$ ($\lambda = 0.7107 \text{ \AA}$) radiations where appropriate.

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