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Ga<sup>3+</sup> ions. Finally, crystal structure or still undetermined efore we can discuss

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. A. SEMILETOV, T. V. HITAR, Kristallogativa Some Proposals for Transformation Mechanisms of the Li<sub>2</sub>ZrF<sub>6</sub>, Trirutile and Na<sub>2</sub>SiF<sub>6</sub> Structure Types: Simple Cation Rearrangements

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Under high pressure, rutile transforms into a structure of the  $\alpha$ -PbO<sub>2</sub> type. In a previous paper (1) we proposed a simple mechanism for this transformation which is illustrated in Fig. 1. We now suggest similar cation displacements to interconvert the Li<sub>2</sub>ZrF<sub>6</sub>, trirutile, Na<sub>2</sub>SiF<sub>6</sub> and columbite structure types.

When  $Li_2NbOF_5$  was reported (2) as being isostructural with  $Li_2ZrF_6$  (3), a picture was made showing its relation to the rutile structure. In Figs. 2a and b, the structures of trirutile and  $Li_2NbOF_5$ are compared; Fig. 3 shows how the  $Li_2ZrF_6$ structure type can transform into the trirutile type if 50% of the cations are shifted in the way







FIG. 1. The rutile structure (upper left) is compared with the  $\alpha$ -PbO<sub>2</sub> structure type (upper right). Below is shown a possible mechanism for the rutile  $\rightarrow \alpha$ -PbO<sub>2</sub> transformation. Cation movements are indicated with arrows.