

Some Proposals for Transformation Mechanisms of the Li_2ZrF_6 , Trirutile and Na_2SiF_6 Structure Types: Simple Cation Rearrangements

JEAN GALY AND STEN ANDERSSON

Service de Chimie Minérale Structurale de la Faculté des Sciences de Bordeaux associée au CNRS, 33-Talence, France

and

Chemical Centre, Department of Inorganic Chemistry 2, Box 740, S-220 07 Lund 7, Sweden.

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Under high pressure, rutile transforms into a structure of the $\alpha\text{-PbO}_2$ 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_2ZrF_6 , trirutile, Na_2SiF_6 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

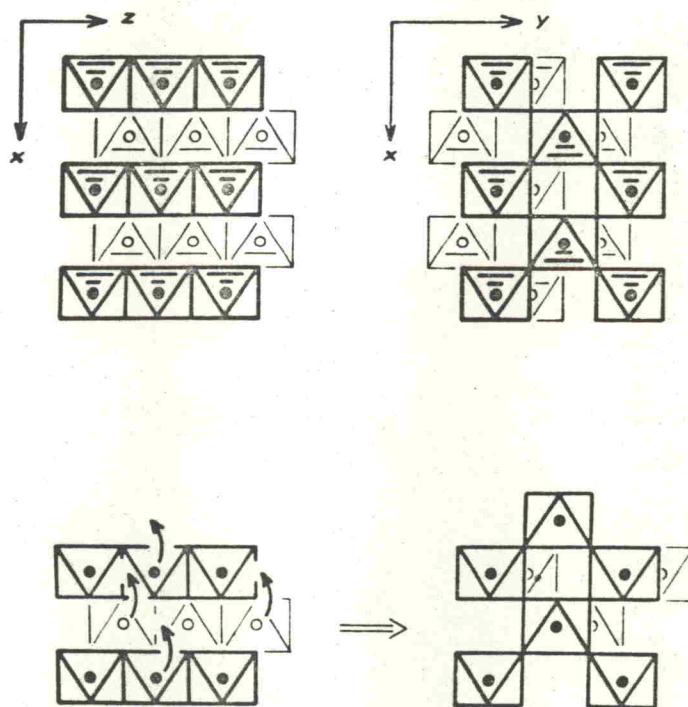


FIG. 1. The rutile structure (upper left) is compared with the $\alpha\text{-PbO}_2$ structure type (upper right). Below is shown a possible mechanism for the rutile \rightarrow $\alpha\text{-PbO}_2$ transformation. Cation movements are indicated with arrows.

Ga^{3+} ions. Finally, crystal structure of still undetermined before we can discuss

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