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

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Under high pressure, rutile transforms into a structure of the α-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. 2*a* 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

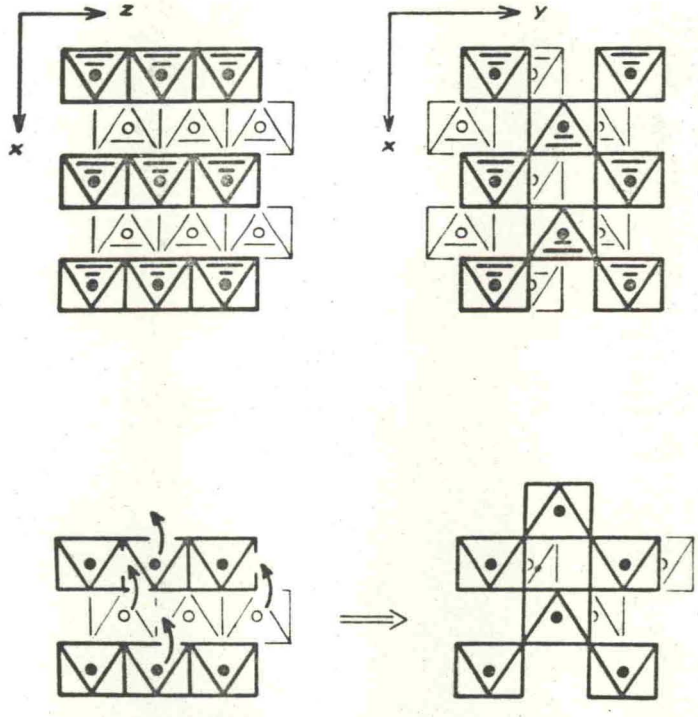

FIG. 1. The rutile structure (upper left) is compared with the α-PbO_2 structure type (upper right). Below is shown a possible mechanism for the rutile → α-PbO_2 transformation. Cation movements are indicated with arrows.