Alkaline Earth Aluminates/Gallates and Perovskites: Two Sides of the Same Coin

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The crystal chemistry of alkaline earth oxoaluminates and gallates covers a large variety of different structure types. However, most of the compounds are based on $[AlO_4]$ - or $[GaO_4]$ -tetrahedra with various degrees of connectivities. The structures of the materials are similar to those observed in silicates (which have been studied in much more detail) and can be classified using the same concepts proposed by Liebau [1].

However, many of the alkaline earth rich compounds can be related to the perovskite structure type as well. For example, the "cyclo-gallate" $Sr_3Ga_2O_6$ containing isolated six-membered $[Ga_6O_{18}]$ -rings can be alternatively regarded as an example for a defect ABO₃-perovskite with 12.5% vacancies in the A-substructure and 25% oxygen vacancies: $(Sr_{7/8}\square_{1/8})(Ga_{3/4}Sr_{1/4})(O_{3/4}\square_{1/4})_3$.

This new concept has been successfully applied to about ten recently determined crystal structures of oxoaluminates/gallates. Using the classical description based on the connectivity of the tetrahedra, the crystal structures look quite different. The "perovskite-approach" offers an elegant way to relate these structures in a simple way.

[1] Liebau F., Structural Chemistry of Silicates, Springer, 1985.

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