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ALKALINE EARTH ALUMINATES/GALLATES AND PEROVSKITES: TWO SIDES OF THE SAME COIN

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In contrast to the great number of investigations aimed to elucidate the phase equilibria in the systems (Ca,Sr,Ba)O-$(Al,Ga)_2O_3$ it is interesting to note that quite recently only a limited number of structural studies have been performed on these materials. This is even more surprising since alkaline earth oxoaluminates, for example, occur in several technologically important processes (sulphate resistant calcium aluminate cements, persistent luminescence materials, refractories etc.).

At a first glance, the crystal chemistry of these compounds covers a large variety of different structure types. However, most of them 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 principally classified using the same concepts that have been proposed by LIEBAU (1985).
On the other hand, many of the alkaline earth rich compounds can be related to the perovskite structure type as well. For example, the "cyclo-aluminate" $Sr_3Al_2O_6$ containing isolated six-membered $[Al_6O_{18}]$-rings can be alternatively regarded as an example for a defect ABO_3-perovskite with 12.5% vacancies in the A-substructure and 25% oxygen vacancies: $(Sr_{7/8}\square_{1/8})(Al_{3/4}Sr_{1/4})(O_{3/4}\square_{1/4})_3$.

This new concept has been successfully applied to the following crystal structures of oxoaluminates/gallates that have been recently determined in our group: $Ca_2Al_2O_5$, $Ca_2Ga_2O_5$, $Sr_3Ga_2O_6$, $Ba_3Ga_2O_6$, $Ba_4Al_2O_7$, $Sr_4Ga_2O_7$, α-$Sr_{10}Ga_6O_{19}$, β-$Sr_{10}Ga_6O_{19}$ and $Sr_{10}Al_6O_{19}$. Using the classical description based on the connectivity of the tetrahedra, these materials look quite different. The "perovskite-approach" offers a simple and elegant way to relate these structures.

LIEBAU, F. (1985): Structural chemistry of silicates. - Springer Verlag, Berlin.