Gallium Substitution in Alumosilicate Halide Sodalites

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In the $Na_8[AlSiO_4]_6X_2$ sodalite system (X = Cl, Br, I) the aluminium atoms were partially substituted with gallium progressively. The synthesised products represented the new composition Na₈[Al_{1-y}Ga_ySiO₄]₆X₂ (0 \leq y \leq 1). Gallium concentrations for different compositions were calculated using X-ray powder data Rietveld refinements and ²⁹Si MAS NMR spectroscopy. The lattice parameters increased [1, 2] linearly from $[AlSiO_4]_6$ to [GaSiO₄]₆ framework matrix. The Al/Ga-O distance was found as an average magnitude [2], which increases with increasing gallium concentration while the Si-O distance remained almost constant at 162.8 pm ($\sigma \sim 2$), 163.4 pm ($\sigma \sim 3$) and 162.6 ($\sigma \sim 2$) for the chloride, bromide and iodide sodalite, respectively. The increasing average tilt of the framework Al/GaO4 and SiO4 tetrahedra led to Na-O and Na-X distances shortening as a consequence of increasing gallium content in the trivalent site of the framework. The degree of framework oxygen s-hybridisation was observed linearly correlated to average T-O distances. In the XRD patterns no clear hints for domain formation of aluminium and gallium enriched parts in the crystals were observed. However, the ²⁹Si MAS NMR spectra showed clearly a non statistical distribution of the different Si-(OT¹₄) surroundings for bromide and iodide sodalites (y ~ 0.30 - 0.70). In the chloride sodalite series, aluminium and gallium were observed statistically distributed throughout the crystals.

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