Single-crystal Structure and Solid-state NMR of Ga$_{2-x}$Sc$_x$O$_3$ ($x = 0.83$)

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Colorless needles of Ga$_{2-x}$Sc$_x$O$_3$ ($x = 0.83$) were isolated during the crystal growth of La$_3$Ga$_3$Sc$_2$O$_{12}$ in a K$_2$WO$_4$ flux. The structure was refined from X-ray single-crystal data: $\beta$-Ga$_2$O$_3$ type, $C2/m$, $Z = 4$, $a = 12.716(4)$ Å, $b = 3.1566(6)$ Å, $c = 5.928(5)$ Å, $\beta = 102.57(3)^\circ$, $V = 232.2$ Å$^3$, $wR^2 = 0.0618$, 429 $F^2$ values, 32 variables. The structure is based on infinite double chains of edge-sharing Sc/GaO$_6$ octahedra running along the $b$ axis. The GaO$_4$ tetrahedra connect these chains by sharing corners and form a three-dimensional framework. The oxygen atoms form a distorted ccp pattern. The $^{45}$Sc NMR spectra confirm the presence of a single scandium site, while $^{71}$Ga NMR data clearly prove the partial occupancy of the scandium site by gallium atoms. The nuclear electric quadrupolar parameters of $^{45}$Sc and $^{71}$Ga are discussed in relation to the crystallographic atomic environments.

Key words: Scandium, Crystal Chemistry, Solid-state NMR