# Rietveld analysis of $Be_3Al_2(SiO_3)_6$ employing high-resolution neutron powder diffraction patterns

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Beryl is one of the most important gem minerals. It is colorless in pure form. However, many different impurities give to beryl its varied coloration. Without these color varieties, beryl would be a rather ordinary gemstone. Emerald, the most precious variety of beryl, is green in color. Aquamarine is the blue variety. In this work, a structural study of beryl has been made using samples from Teófilo Otoni, Minas Gerais, Brazil. Neutron powder diffraction patterns were measured on the neutron diffractometer Aurora, recently installed on the IEA-R1 research reactor at IPEN-CNEN/SP. Although IEA-R1 is a low-flux reactor, installation of both a position-sensitive detector (PSD) and a double-bent focusing silicon monochromator has turned possible to design the new instrument as a high-resolution powder diffractometer (HRPD). Two samples of beryl have been studied. One that is blue in color we have identified as an aquamarine. Other that is pale-blue in color we have simply called beryl. Powdered samples have been analyzed by program GSAS which employs the Rietveld method in the analyses. Structural as well as anisotropic thermal parameters were refined in order to determine the right chemical compositions of the samples. During the analyses we have introduced impurities that are commonly encountered in blue beryl. The final results of the analyses are the following: in both samples Fe and Na were identified as impurities; the final compositions for aquamarine and beryl are $Be_3Al_{1.83}Fe_{0.17}Na_{0.03}(SiO_3)_6$ and $Be_3Al_{1.89}Fe_{0.11}Na_{0.25}(SiO_3)_6$, respectively. Two of the most common numerical criteria of fit given in the output of GSAS, R-pattern ($R_P$) and R-weighted pattern ($R_{WP}$), resulted equal to 0.024 and 0.034, for aquamarine, and 0.022 and 0.032, for beryl.