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DETERMINATION OF THE CELL PARAMETERS OF β -QUARTZ AT 1003 K BY NEUTRON MULTIPLE DIFFRACTION

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In this work, neutron multiple diffraction (NMD) data was employed for the determination of the parameters a and c of the β -quartz hexagonal cell at 1003 K. An experimental 00.1 β -quartz NMD *Umweg* pattern has been used for the determinations. During the indexing of the β -quartz pattern it was verified that most of the peaks could be classified as either *good for the determination of the parameter a* or *good for the determination of the parameter c*. With such a classification, it became possible to employ an iterative method for the determination of both parameters. To attain this purpose, a method named *relative method*, using azimuthal angular differences between two selected peaks, was developed. The values obtained for both parameters, in this method was found by comparing the azimuthal angular differences with indexing theoretical diagrams. An iterative and alternate process was applied in order to obtain the values of the parameters. In this process, the value obtained for one of the parameters is used in the determination of the other parameter. The iterative process continues until both parameters converge. The values of the parameters obtained by the *relative method* were: $a = 4,99646 \pm 0,00058 \text{ \AA}$ and $c = 5,46116 \pm 0,00044 \text{ \AA}$.

Keywords: Neutron multiple diffraction, Hexagonal cell parameters, Beta quartz.

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