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Study of a highly crystalline Y₂O₃ sample by Rietveld and Pair Distribution Function Analysis

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An Y₂O₃ highly crystalline sample, used as standard reference material for X-ray diffraction experiments, was studied by Rietveld and Pair Distribution Function analysis. The structural parameters obtained using Rietveld refinement, such as cell parameters, atomic positions and isotropic atomic displacement factors were compared previous studies and literature data. Besides that, the high-energy x-rays scattering data, collected at the LNLS-XDS beamline, allowed perform pair distribution function (PDF) analysis. The data was collected in Bragg-Brentano geometry and using a scintillation punctual detector, with 20 keV energy radiation, reaching a Qmax resolution of 20.05 Å⁻¹. The PDF analysis showed that the SRM exhibits a very large structural coherence length, no structural disorder and can be considered perfectly ordered over very large interatomic distances, as expected from a standard reference material.