Structural solution of the high-pressure polymorph of scintillating β-$MgMoO_4$ by means of single crystal x-ray diffraction

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Ionizing radiation and particle physics scintillating detectors, tunable lasers, or optoelectronic devices are some of the applications in which molybdates can be found. The reason is their high light yield emission when hit by γ-particles or x-rays. Unfortunately, their emission shows long scintillation times that range from 12−15 μs. This drawback has been tried to be palliated up to some extent by the tune of the optical properties of molybdates using high pressure or high temperature. However, molybdates do not only present a vast polymorphism at ambient conditions but also under extreme conditions. The case of $MgMoO_4$ is a particularly interesting one since it crystallizes either in a cuproscheelite-type polymorph ($P\bar{1}$) named α-$MgMoO_4$ or in a monoclinic polymorph ($C2/m$) named β-$MgMoO_4$. On top of that the β polymorph undergoes at ambient pressure two phase transitions to an incommensurate and a hexagonal phase at 640 and 770 K, and at ambient temperature a phase transition to an irreversible and unknown structure at 1.4 GPa [1].

In this work we focus on the structural solution of the high-pressure polymorph of β-$MgMoO_4$. According to a previous Raman spectroscopy study this pressure-induced phase transition involves a coordination increase from 4 to 6 of the MoO_n polyhedra and involves either no change of the symmetry elements of the crystal or the loss of the centering of the unit-cell. Our structural solution by means of single-crystal x-ray diffraction performed at the ID15 beamline of the ESRF unveils an isosymmetric phase transition in wich the Mo polyhedra increase their coordination from tetrahedral to octahedral with half of the Mg and Mo polyhedra aligning two of their distances along the [001] direction. Our result has allowed us to perform *ab initio* calculations to reinterpret the previously published Raman spectroscopy data [1].

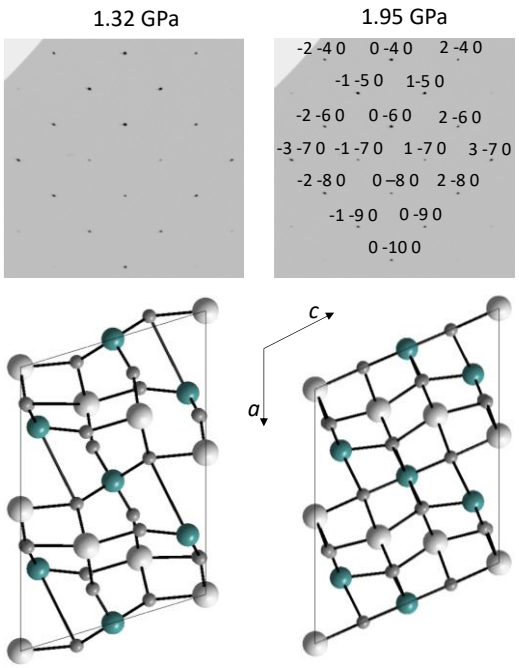

Figure 1. Section of the reconstructed reciprocal space and solved structures at 1.32 GPa (β-$MgMoO_4$, $C2/m$) and 1.95 GPa (high-pressure polymorph, $C2/m$). The presence of the $h+k = 2n$ extinction condition persists in the high-pressure phase rejecting the previously proposed $P2/c$ space group.

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