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In this study we investigate the α -phases of La, Ce, Pr and Nd tri-tungstates under high pressure. These compounds showed amorphization when they are under pressure, which is partially reversible when the pressure is released, as in the α -phases of Nd, Tb and Eu molybdates [1]. High-pressure powder X-ray diffraction experiments have been performed at room temperature in the MALTA X-Ray Diffractometer (Xcalibur from Oxford Diffraction, Universidad Complutense de Madrid). The samples have been prepared by a conventional solid-state reaction of La_2O_3 , $\text{Ce}_2(\text{CO}_3)_3$, Pr_6O_{11} , Nd_2O_3 . In this work, we have applied a new alternative method for treating distorted structures by means of symmetry mode analysis (for the displacively distorted α -phase from the tetragonal scheelite structure) performed using the program AMPLIMODES, developed in the Bilbao Crystallographic Server [2], and the Rietveld refinement of the amplitudes of such symmetry modes using the Fullprof program [3]. The proposed studies have been complemented with theoretical *ab initio* total-energy calculations where we have obtained an anomalous expansion of the cell parameters.

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Keywords: high pressure amorphization, rare earth tungstates

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Non ambient crystallographic studies of dithienylethene optical molecular switches

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Dithienylethene compounds are of significant interest due to their photochromic properties. These compounds undergo electrocyclic ring closure and opening reactions when irradiated and are stable to thermal reversion and fatigue, making them ideal for applications within the area of the molecular memories and switches [1]. More recently interest has developed with regards to their solid state properties, demonstrating interesting and unique behaviour for photochromic compounds such as capacity for single crystal transformations between the open and closed form and the ability to exert mechanical force upon an object upon irradiation [2-3].

Therefore we report the structures of a series of new dithienylethene based systems and report on their solid state behaviour, demonstrating several reversible single crystal to single crystal transformations to high levels of conversion. We also report an investigation into the behaviour of four dithienylethenes under elevated pressure, ranging from 0 to 10 GPa in the single crystal and report interesting changes in conformation and intermolecular packing forces.

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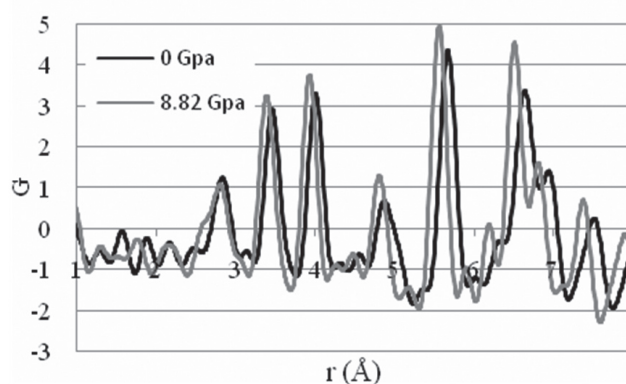
Investigating the Structure of BaTiO₃ using Pair Distribution Function Analysis of High Energy X-ray Scattering Data

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Barium titanate (BaTiO₃) is a perovskite ferroelectric oxide that undergoes phase transitions under changes in pressure. It has been one of the most exhaustively studied ferroelectric materials since its discovery, and many would consider it the prototype. At room temperature and pressure it possesses a tetragonal structure, which arises due to the elongation of the cubic unit cell along the [001] direction. At high pressures, BaTiO₃ undergoes a phase transition to what is generally believed to be a cubic structure. There is some debate on the exact structure of this high pressure phase and the exact transition pressure; this is because spectroscopic signals indicating the Ti atom is still off the ideal position persist even though no distortion can be measured in the unit cell parameters.

In this work we are using the pair distribution function (PDF) analysis method to further study these phase transitions. The PDF is obtained *via* the Fourier transform of the total scattering pattern and yields more information than standard Rietveld analysis as Bragg and diffuse scattering are analysed together without bias, revealing the short and intermediate range order of the material regardless of the degree of disorder. PDF analysis has been used to study the structure of Barium Titanate over a range of pressures around the expected phase transition from tetragonal to cubic structures.

Gr for BaTiO₃ under pressure



Keywords: high-pressure, phase transition, pair distribution function.

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Modeling of disorder in BaThF₆; anharmonic displacement parameter from high-pressure data

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Binary and ternary fluorides with the tysonite structure are extensively studied due to their superionic conductivity [1,2] and their optical properties in the presence of rare earth elements [3]. They