

m30.p15**Polymorphism in 4-methoxy-3-nitrobenzaldehyde**Sara Wishkerman^a, Joel Bernstein^a, Peter W. Stephens^b^aDepartment of Chemistry, Ben-Gurion University of the Negev, P.O. Box 635 Beer Sheva, Israel, 84105, ^bDepartment of Physics & Astronomy, State University of New York, Stony Brook, New York 11794 USA, E-mail: saraw@bgu.ac.il.**Keywords: polymorphism, powder diffraction, single crystal X-ray diffraction**

The increasing importance of polymorphism - the ability of a solid state to exist in at least two different arrangements of the molecules in the lattice - is due to the correlation between the structure and properties of solids. In particular, the identification and characterization of the desired polymorphic form is necessary in order to ensure reliable and robust manufacturing processes of a substance.

4-methoxy-3-nitrobenzaldehyde (MN) has been used in nucleophilic aromatic substitution to synthesize compounds of benzaldehydes with nitro and amino functionalities. These latter compounds are important in the pharmaceuticals industry, especially in therapy for Parkinson's disease and certain cancers. In 1990 Kuhnert-Brandstätter and Sollinger identified three polymorphs of MN with microscope hot stage, DSC and IR spectroscopy, but apparently did not carry out any X-ray diffraction studies.¹ In our investigation two of the three earlier reported polymorphic forms of MN have been reinvestigated and fully characterized by a variety of methods including variable temperature powder X-ray diffraction (PXRD), vibrational spectroscopy (Infrared and Raman), calorimetry (DSC) and optical microscopy.

A third form, Form γ , was observed only transiently in the DSC and transforms to Form α upon cooling. Differences of DSC thermograms which were carried out with different cooling rates suggest a thermodynamic/kinetic competition in the crystallization from the melt. The crystal structures of these two forms have been solved: one by single crystal methods and the second from synchrotron powder diffraction.

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m31.p01**Analysis of structural electrical and optical properties of Sol-Gel titanium oxide (TiO₂) thin films**Raouf Mechiakh^a, F. Meriche^b, R. Gheriani^c, R. Bensaha^a, R. Kremer^b, A. Boudrioua^b^aCeramics Laboratoire, Université Mentouri Constantine, Algeria. ^bLaboratory Materials Photonic Optics and Systems CNRS UMR 7132, University of Metz and Supelec 2 street E Belin 57070 Metz, France. ^cUniversity of Ourgla, Algeria. E-mail: Raouf_mechiakh@yahoo.fr**Keywords: thin-films, TiO₂, sol-gel**

Titanium dioxide (TiO₂) has been attracting much interest for a wide range of applications such as dye sensitized solar cells [1], photocatalysts [2], electrochromic display devices [3] and planar waveguides [4]. It is known that titanium dioxide has three crystalline modifications-rutile (tetragonal), anatase (tetragonal) and brookite (orthorhombic) [5]. In this study, we interested ourselves in the analysis of structural electrical and optical properties of Sol-Gel titanium oxide thin films. TiO₂ thin films were prepared by a sol-gel dip-coating process using titanium alkoxide. We used several experimental techniques to monitor the structural evolution and the electrical properties resulting from different annealing treatments and different dipping iterations: X-Ray Diffraction, Raman Spectroscopy, scanning electron microscopy, m-Lines, IR and UV Spectroscopy and optical microscopy. DRX and Raman analysis of our thin films of TiO₂ shows that the titanium oxide can transform from the amorphous state into (crystalline) anatase, an anatase-brookite mixture, respectively, with increasing treatment temperature and/or number of dipping iterations. Calculation of the size of the titanium oxide nano-crystallites with Scherrer's formula gives sizes in the range 6 to 33 nm. The characterization electric show that the interface of our layer with a behavior in matter semiconductor of type n, and the leakage current de fuite be less significant when one increase the number of layer, this loss of current perhaps allot with density high of pore, plus the thickness be large plus the structure be porous. The refractive index (n) and porosity (p) is found to be independent of thickness.

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